

SUBMERGED ARC WELD MODELLING

FINAL REPORT

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TABLE OF CONTENTS

Abstract-----	1
List of Figures-----	2
List of Tables-----	2
Introduction-----	3
Welds Analyzed-----	7
Thermal Modelling	
(A) Double Ellipsoid Modelling-----	9
(B) Compound Double Ellipsoid Modelling-----	9
(C) Discussion of "Bay" Thermal Modelling-----	17
HAZ Hardness Computations and Measurements-----	18
Preheat Computations-----	21
Microstructure Computations-----	22
Addition of Fusion Zone Microstructure Algorithm-----	23
Papers and Presentations Arising From this Contract---	23
Acknowledgments-----	23
References-----	24
Appendix A	
Appendix B	
Appendix C	

SUBMERGED ARC WELD MODELLING

ABSTRACT

Progress in modelling the submerged arc welding process to predict thermal history and HAZ properties: microstructure, hardness, and cracking threshold is reported in this presentation. Included in the report is an investigation of thermal changes in the "bay" region of a 3kJ/mm bead on plate (25 mm thick, no preheat) weld. The peak temperature and retention time above 1000 C distributions are reported for this welding situation. The results are rationalized in terms of the compound ellipsoid heat source model used to make the computations. The significance and limitations of these computations in view of the submerged arc solidification morphology demonstrated in a recent investigation by Barlow [1] is discussed.

Beyond thermal history, software for predicting HAZ microstructure, hardness and the preheat necessary to prevent cold cracking is presented. Microstructure and hardness computations for the 3kJ/mm weld are included. In addition, parametric variations as the welding input parameters (current, voltage, preheat, ambient temperature, and welding speed) change are presented to demonstrate the advantages and potential of weld modelling. The significance and limitations of these computations for welds that contain a bay are discussed.

Several papers have been published and presentations delivered during the course of this work. They are listed and discussed in the presentation. The potential of weld modelling for metallurgical and welding engineering applications is discussed. Future developments are suggested. In particular the possibility of integrating recent methods of computing the microstructure and properties of weld metal into the Carleton computational system is mentioned. Further work beyond the terms of this contract is suggested.

LIST OF FIGURES

- Figure 1 Double ellipsoid configuration used to model welding heat sources. For details see reference 5.
- Figure 2 Four welds submitted for analysis in this investigation -- (A) 350WT (STRAND), (B) BS4360, (C) LT60, (D) 350WT (CAB).
- Figure 3 FEM mesh with FZ and HAZ profiles in position. Location of paths 1-2-3-10-11, and 5-2-12 through the bay region selected for study -- see Figures 4,5, and 6.
- Figure 4 Peak temperature distribution along path 1-2-3-10-11. See Figure 3 for definition of the path.
- Figure 5 Peak temperature distribution along path 5-2-12. See Figure 3 for definition of the path.
- Figure 6 HAZ peak temperature distribution generated with the conventional theory of Ion et al [4]. Note that a such an analysis assumes no bay and is therefore included only for comparison purposes.
- Figure 7 Nodal values of the retention time above 1000 C for a 3kJ/mm weld.

LIST OF TABLES

- Table 1 Off-shore steels and compositions
- Table 2 Submerged arc welding parameters and workpiece dimensions
- Table 3 Cooling time computations for a 3kJ/mm submerged arc weld
- Table 4 Comparison of computed and measured HAZ width dimensions
- Table 5 HAZ hardness levels for CANMET off-shore steel welds
- Table 6 Measured and computed HAZ periphery hardness values
- Table 7 Computed HAZ weld line microstructures
- Table 8 Cross-sectional dimensions of CANMET welds
- Table 9 Melting points and eutectoid temperatures for CANMET steels

SUBMERGED ARC WELD MODELLING

INTRODUCTION

Over 80% of all steel tonnage is welded. It is apparent that welding is a crucial fabrication process in manufacturing industry and yet it is not at all well understood. Because of this weld modelling has been slow to develop and welding has remained largely a skill practiced by talented artisans. Engineering control to ensure sound welds is based to a great extent on experience and on the results of various critical tests such as the implant or wide plate procedures.

Beyond experience and critical testing, microstructural examination and characterization of the heat-affected-zone (HAZ) has added a great deal to the understanding of the behavior of the welded joint. The same can be said of the fusion zone although weld metal microstructure formation is somewhat more complex. Nevertheless it is still fair to say that unfavorable microstructures and suspect joint properties cannot be predicted unless there is similar documented experimental experience available to the metallurgist or engineer faced with the task of designing welding procedures and conditions.

Weldability is the term often applied to characterize the response (joint quality) of a material to the welding process. This implies that a material can be indexed according to its weldability which misrepresents reality. Because there are several independent and interacting dependent parameters that determine the behavior of a welded joint, weldability is not easily defined. In view of this, material characteristics such as weldability and formability have recently been labeled "systems properties". In this author's view a systems interpretation is an important contribution that should help considerably with the weldability concept.

While the arguments of the last paragraph are interesting academically they do little to rationalize the task of specifying appropriate welding parameters for a given welding situation. At the present time the principal prerequisite for this task is experience. Consequently "welding engineers" must have considerable experience in fabrication technology before they can accept the responsibility of fixing welding parameters and conditions. They are critical to any industry that depends on welding as a manufacturing process and yet the availability of personnel with this kind of experience is often limited.

Mathematical modelling is at least a partial alternative to experience. Having said this it is recognized that models always contain assumptions and approximations that limit the significance of the computations. Therefore, models can only be viewed as an aid and by no means a complete substitute for judgment and experience. However, modelling in the grasp of a skilled metallurgist or welding engineer can provide considerable insight that would otherwise be unavailable. To appreciate the importance of modelling it is only necessary to visualize the difficulties that would be encountered if it were necessary to make strain measurements every time stress levels were needed by an engineer. The fact that stress, strain, and displacements can be computed from elasticity models with appropriate boundary conditions is of enormous importance.

Ideally given the input welding parameters (current, voltage and welding speed), the initial conditions (preheat) and the boundary conditions (ambient temperature), it would be of considerable value to be able to compute the mechanical properties of the HAZ and WM, and the threshold conditions for crack formation. The converse problem is of equal or perhaps even of more importance i.e. given the properties necessary for the joint to perform in service what are the appropriate welding parameters.

Yet modelling the welding process has received relatively little attention until recently. Presumably this situation prevailed because of the complexity of the arc/weld pool interaction. Even now details of the physics of the arc and the magnetohydrodynamics of the weld pool are not well understood and therefore the process cannot be modelled with certainty.

Several heat source approximations have been applied beginning with the point source originally proposed by Rosenthal [2]. Beyond this a disc heat source has been proposed by Pavelic [3] and by Ion et al [4]. The most advanced heat source until this work is the so-called double ellipsoid (Figure 1) proposed by Goldak et al [5].

The double ellipsoid is a shape that approximates that of the weld pool. A Gaussian power distribution is imposed on this shape. The high power density at the origin is said to reflect the intensity of the arc at the center. The power intensity then decreases near the edges of the pool where stirring effects are expected to be less. Melt out beyond the boundaries of the ellipsoid establishes the molten pool and ultimate size of the fusion zone.

It is evident that the ellipsoid is not a heat source model in the traditional sense but is really a combined heat source/weld pool model. It is, however, the best that can be done in the absence of more detailed knowledge of the arc and molten pool dynamics. This model is appropriate for normal welds where the weld metal zone is ellipsoidal in shape. However, the molten pool in many welds is depressed by arc pressure and deep penetration

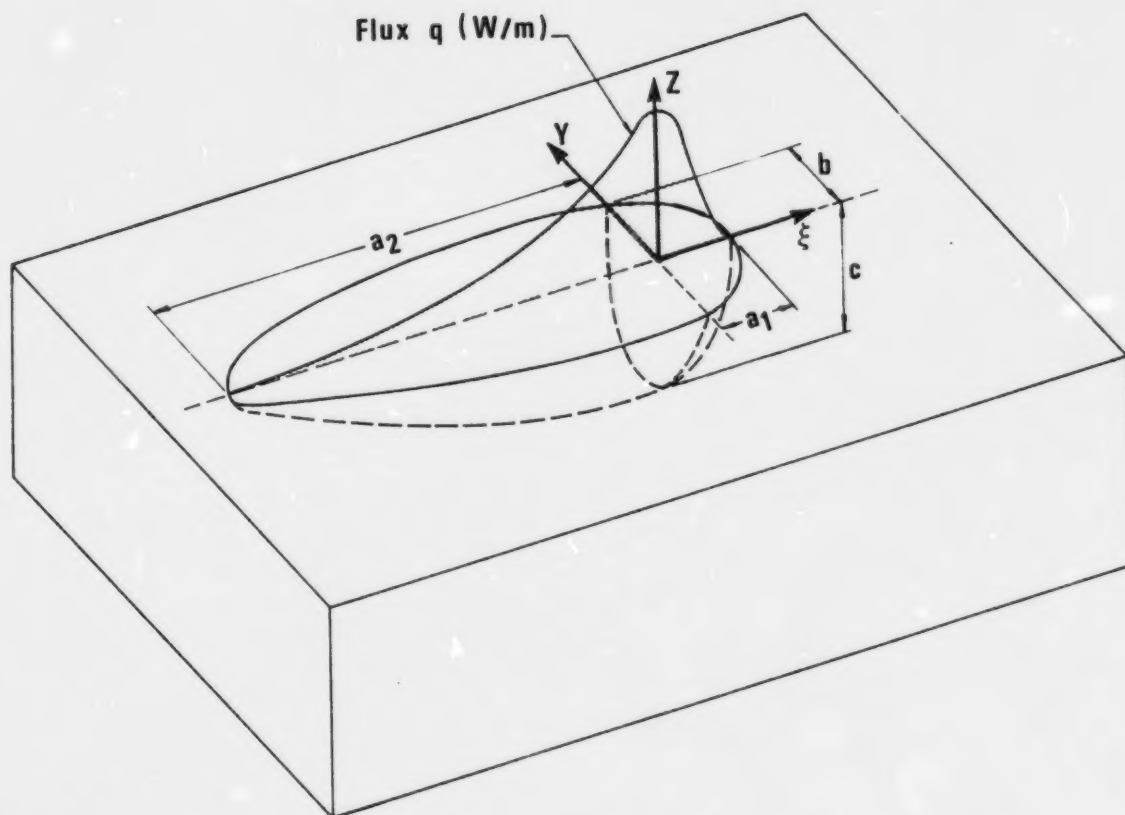
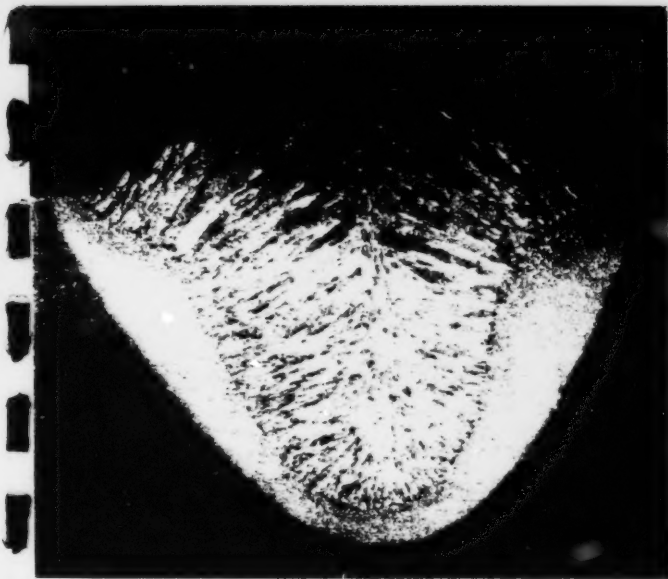
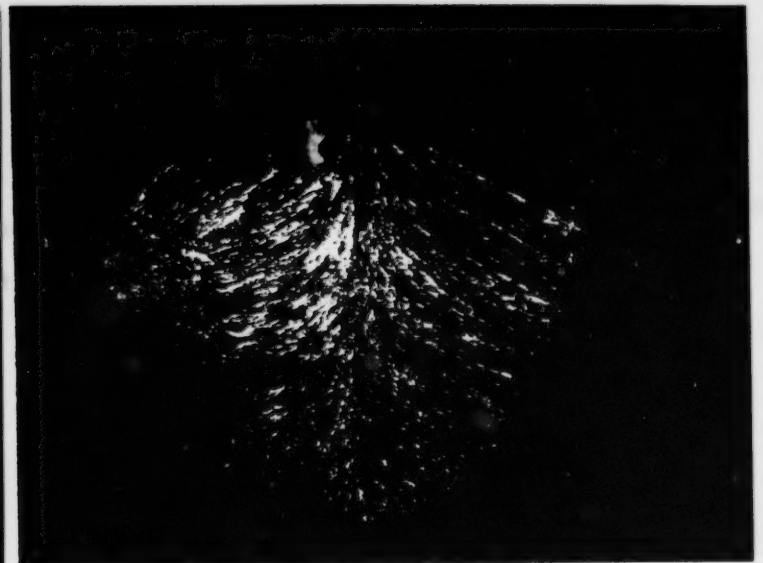


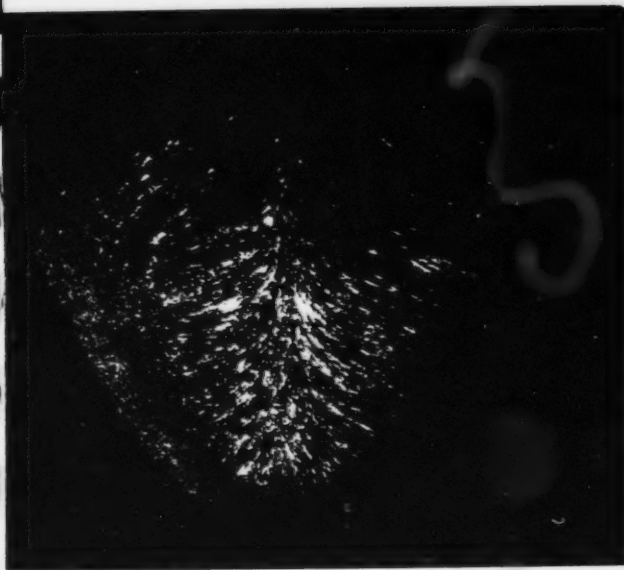
Figure 1 Double ellipsoid configuration used to model welding heat sources. For details see reference 5.



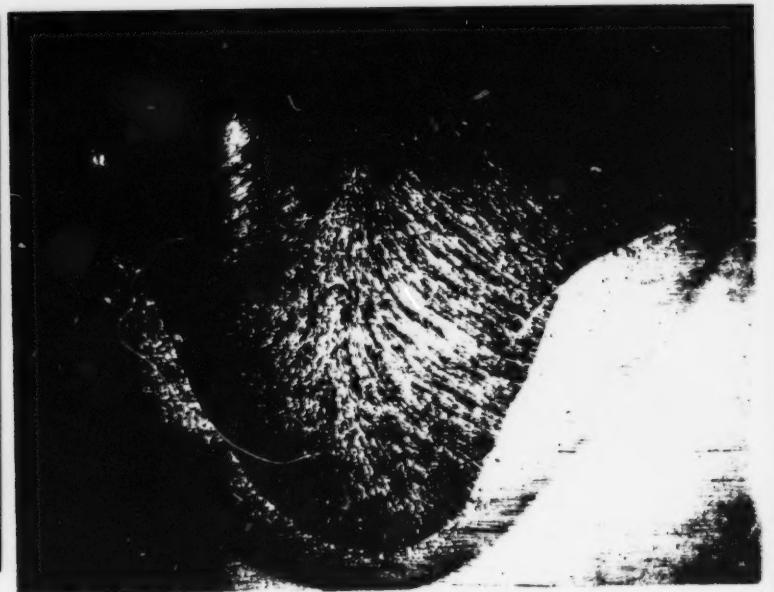
A



B



C



D

Figure 2 Four welds submitted for analysis in this investigation
-- (A) 350WT (STRAND), (B) BS4360, (C) LT60, (D) 350WT (CAB).

occurs. In this case a bay forms such as those shown in Figure 2. Because of the inherent shape of the double ellipsoid, it is not possible to model the bay area of a weld. For some purposes this may not be important. For example it probably makes little difference in the 800/500 C cooling time. On the other hand the retention time above 1000 C is likely changed considerably in the bay area because of shape effects. This increases austenitic grain growth which, in turn, leads to higher hardenability structures.

Modelling a weld with a bay shape is not an easy task. Certainly what is reported in this presentation is the first attempt anywhere to predict thermal changes in the bay region from the input welding parameters. This claim must be qualified to include work from the Welding Institute where the cross section is profiled, meshed and the fusion boundary set to the melting point. The heat input is then allowed to flow from the boundary. This, however, is a considerable approximation to reality. It does not account for the dynamics of the heat source. In addition, it is not clear to this investigator that the computations are unique. Nevertheless, such computations are interesting and useful, and certainly occupy a place in the development of bay modelling.

At the outset of this work it was suggested that compound double ellipsoids might be used to model the bay region. This, in effect, amounts to a situation where the input power is distributed over two double ellipsoids located one above the other. The results of computations with this configuration are presented in this report. Also included is a discussion of the limitations of such computations.

Beyond thermal modelling the application of semi-empirical auxiliary models for computing HAZ hardness, microstructure, and crack formation threshold is investigated. In particular they are examined for significance to situations where a weld contains a bay. The entire computational system is then discussed in terms of observations and measurements for such welds. Finally the possibility of adding a weld metal microstructure algorithm based on the work of Bhadeshia [6] is discussed.

WELDS ANALYZED

Four potential off-shore microalloy steels containing 3kJ/mm submerged arc welds were obtained from CANMET for investigation. The steel designations and compositions are contained in Table 1. The welding parameters used to make this weld are contained in Table 2. Cross sectional configurations are shown in Figure 2.

TABLE 1

CANMET OFF-SHORE STEELS AND COMPOSITIONS

STEEL	C	Mn	Si	S	P	Cr	Ni	Mo	V	Nb	Ti
350WT (CAB)	.15	1.44	.24	.005	.015	.040	.225	--	.06	.02	.01
BS4360	.14	1.33	.37	.01	.02	.015	.010	.010	--	.027	--
LT60	.12	1.29	.272	.008	.015	.151	.135	.010	.053	.039	--
350WT (STRAND)	.07	1.35	.286	.004	.015	.241	.255	.010	.068	.022	.01

STEEL	Al	Cu	Sn	N (PPM)
350WT (CAB)	.015	.015	.005	--
BS4360	.03	.032	.001	73
LT60	.029	.159	.001	70
350WT (STRAND)	.040	.008	.001	62

TABLE 2

SUBMERGED ARC WELDING PARAMETERS AND WORKPIECE DIMENSIONS

Current (Amps)	800	Wire Diameter (mm)	4
Voltage (Volts)	35	Electrode Extension (mm)	32
Travel Speed (mm/s)	9.33	Workpiece Length (mm)	500
Energy Input (kJ/mm)	3	Workpiece Width (mm)	350
Electrode Polarity	DC+	Workpiece Thickness (mm)	25

THERMAL MODELLING

(A) Double Ellipsoid Modelling

In the first instance a conventional double ellipsoid was used to model the heat source. The results of these computations are not terribly interesting because the bay area is not modelled. However, it is interesting to compare the 800/500 C cooling time computations with measured values and with point source calculated values (Table 3). The differences are not great especially in view of the fact that microstructural and physical property changes take place over about three orders of cooling time magnitude. In addition it should be noted that bay modelling changes the cooling time almost not at all.

TABLE 3

COOLING TIME COMPUTATIONS FOR A 3 kJ/mm SUBMERGED ARC WELD

METHOD	COOLING TIME (S)	COMMENTS
Measured	16 - 20	Kohn and Jones[7]
Double Ellipsoid	16.6 - 19.6	This investigation
Adams Point Source	15.8	Rosenthal Approximations[8]
Kohira Point Source	16.1	Allowance for surface losses[8]

(B) Compound Double Ellipsoid Modelling

To achieve a deep penetration profile a second smaller ellipsoid was positioned directly below the primary ellipsoid. Power from the heat source was then proportioned between the two ellipsoids. Several trial runs were required before a bay shape was achieved (Figure 3). In particular it seems that most of the arc power (80%) must be assigned to the larger upper ellipsoid before a bay is formed. This is a surprising result. At the same time the general shape fails when the power level to the lower ellipsoid falls below 20%. There seems to be a very narrow window for the power distribution between the two ellipsoids.

Over and above the power distribution, the ellipsoid axes (Figure 1) must be fixed by the analyst. Fixing these dimensions is not a terribly difficult task for a weld that does not contain a bay shape i.e. a relatively shallow configuration. However, there are a great many combinations in the case of compound ellipsoids and

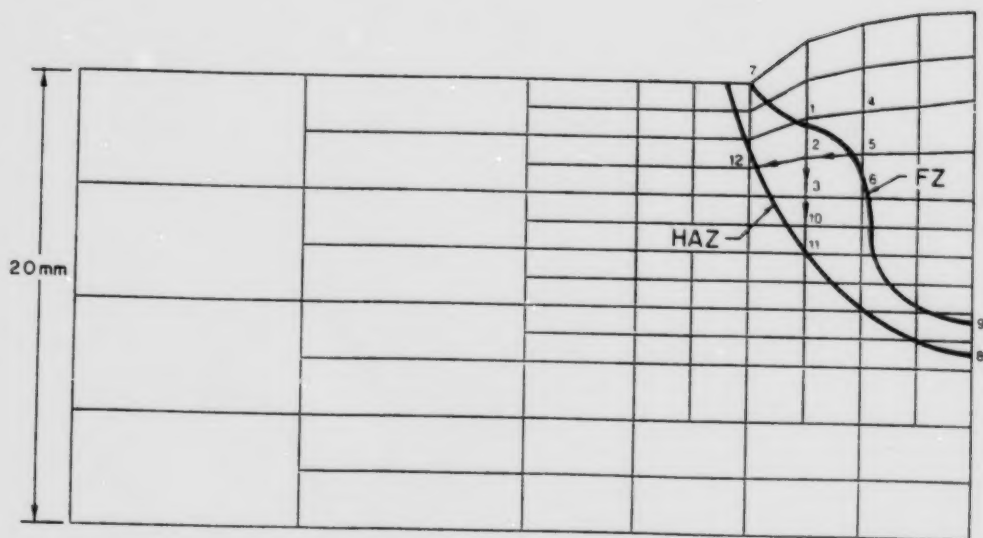


Figure 3 FEM mesh with FZ and HAZ profiles in position. Location of paths 1-2-3-10-11, and 5-2-12 through the bay region selected for study -- see Figures 4,5, and 6.

the task as is not easy. Dimensions somewhat less (usually about 10%) than those of the fusion zone are selected for trial purposes. Melt out establishes the fusion zone boundaries. After initial trial computations the calculated boundaries are compared with cross-sectional measured (metallographic techniques) fusion zone boundaries. If the two are not consistent the ellipsoid dimensions are adjusted.

After several trial computations the dimensions of a_1 , b and c were all set to 6.25mm. The a_2 dimension was set to 12.5mm. A sphere of radius 5mm was used for the lower ellipsoid, positioned 7.5mm below the surface. A sphere is not an unreasonable approximation in this case because it is known that where there is deep penetration the lower part of the cavity is less elongated than the upper volume.

These dimensions were based on metallographic measurements from the 350WT (CAB) weld shown in Figure 2. It is clear that even though the four welds in this Figure are supposed to be identical (i.e. the welding conditions are the same in all cases) they are not consistent. For one thing they are not all symmetrical. In addition, measurements would seem to suggest that as the carbon content increases there is some increase in the size of the fusion zone (see Appendix A).

Of the four welds in Figure 2 the 350WT (CAB) weld is the most symmetrical and therefore it was selected for study. Even though the computations are confined to this particular weld, they probably can be applied to the CANMET other welds or indeed to any 3kJ/mm weld provided the fusion zone boundary is used as a reference position. Some allowance is undoubtedly necessary for inconsistent HAZ widths (side to side) when there is asymmetry. However, this is not considered a serious situation.

The weld profile (FZ and HAZ boundaries) eventually computed is shown in Figure 3. The boundary positions do not match exactly the real weld profiles (Figure 2). However, the agreement is reasonable and, therefore, computed thermal changes in the bay region can be applied (with some allowance) to all 3kJ/mm steel welds. At the same time some of the phenomenological information distilled from the computations is both interesting and significant.

One of the principal differences between the bay region and the rest of the HAZ is grain size. This depends to a great extent on peak temperature and on the retention time above 1000 C, the thermal domain where austenite grains become active and grow. Shown in Figure 4 is the peak temperature distribution along path nodes 1-2-3-10-11. On average the peak temperature spacing along this path is about 145 C/mm. Of course this is approximate since the distribution is a curve. The perpendicular distribution along path 5-2-12 is shown in Figure 5 and the peak temperature spacing along this path is about 165 C/mm. It is interesting to note the convex shape of this curve, presumably because the path is not

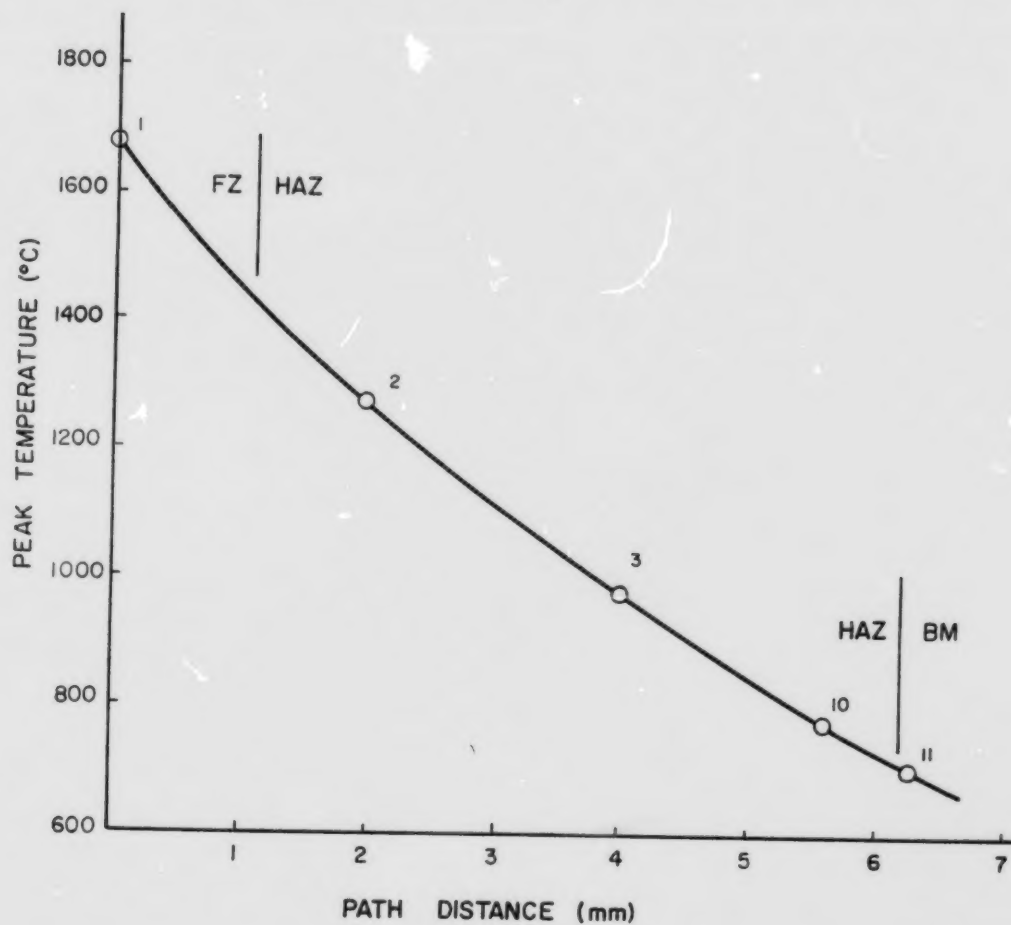


Figure 4 Peak temperature distribution along path 1-2-3-10-11.
See Figure 3 for definition of the path.

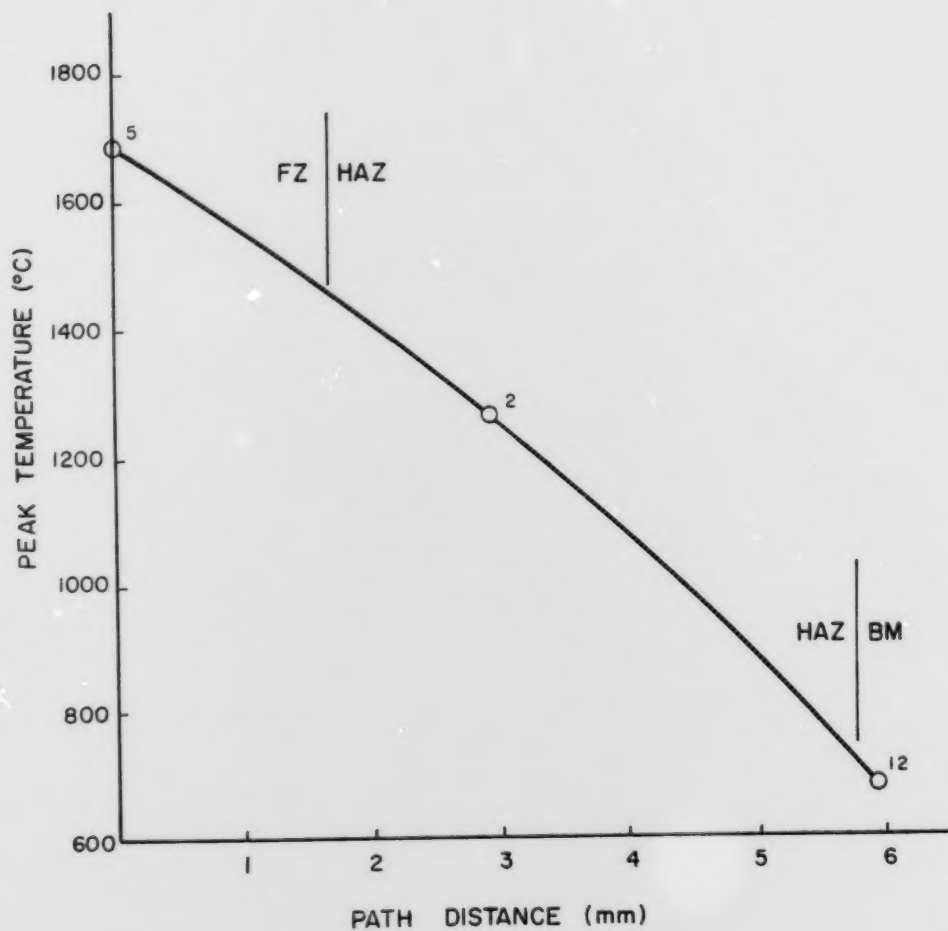


Figure 5 Peak temperature distribution along path 5-2-12. See Figure 3 for definition of the path.

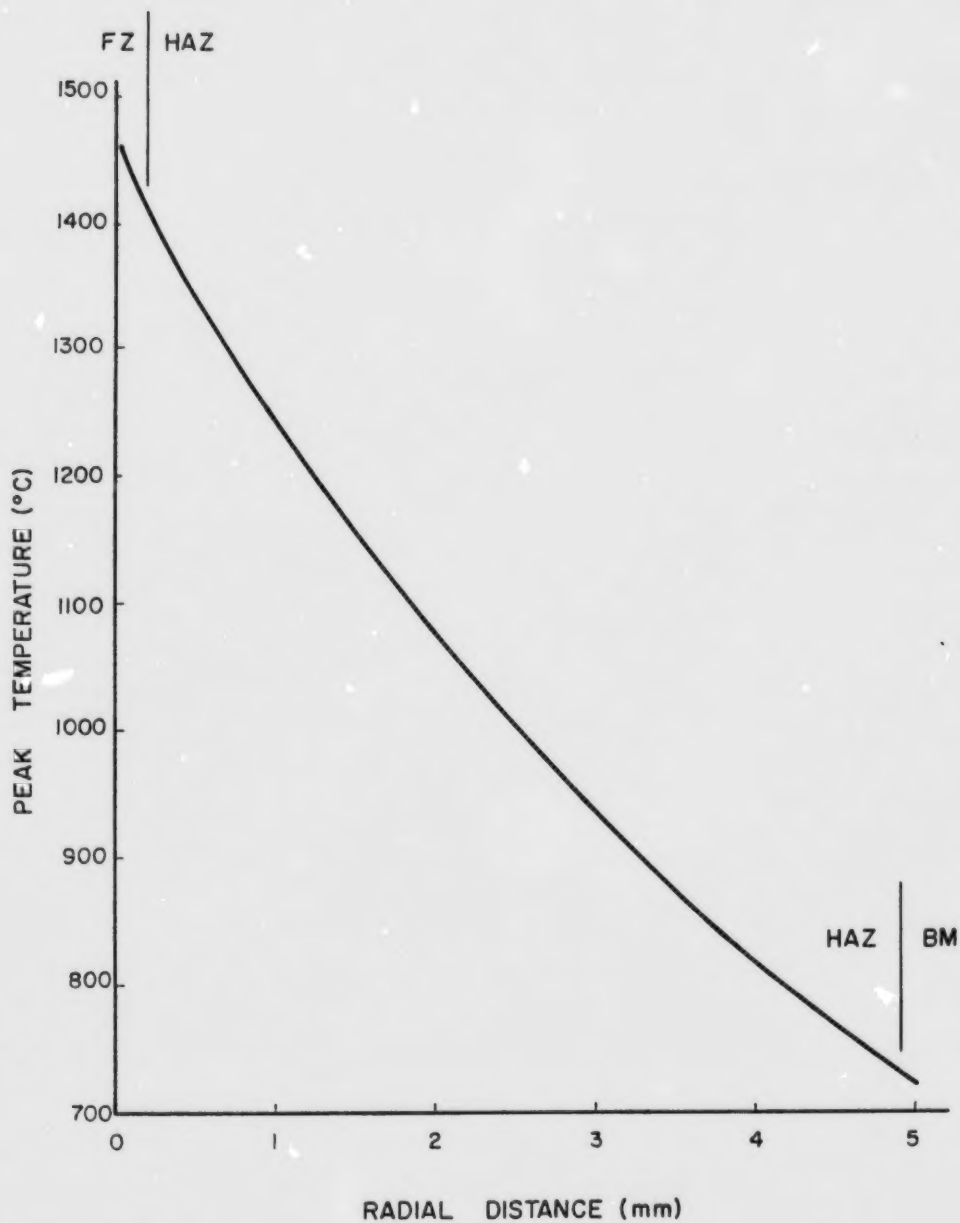


Figure 6 HAZ peak temperature distribution generated with the conventional theory of Ion et al [4]. Note that a such an analysis assumes no bay and is therefore included only for comparison purposes.

normal to the fusion boundary.

The peak temperature spacings computed with FEM may be compared with the spacings obtained from the conventional theory of Ion et al [4] as shown in Figure 6. In this case a spacing of about 140 C/mm is calculated along any radial path from the centerline. The boundary shapes in this model are semi-circular which, of course, precludes the possibility of a bay region. As expected conventional theory underestimates peak temperature spacing.

Some evaluation of the accuracy of the computations can be made by comparing the distance from the fusion line to the HAZ boundary. The assumption is that the fusion boundary represents a peak temperature below which the base metal remains intact and the HAZ boundary represents a peak temperature of A_E . The melting temperatures and the A_E temperatures for the four off-shore steels of this investigation, calculated from empirical relationships documented by Ion et al [4] are listed in Appendix A. A value of 710 C was taken for the eutectoid temperature of the 350WT (CAB) material. The fusion boundary peak temperature was taken to be 1450C even though the computed melting point is 1530 C for this material. It is well known that the melting point does not represent the fusion zone boundary. To begin with two phase effects suggest a lower temperature maybe the solidus. However, this a matter of some debate. Recent Gleeble tests by Bowker [9] suggest a peak temperature of 1450 C and that is what is used in this investigation.

By applying temperatures of 1450 C to the fusion boundary and 710 C to A_E the HAZ width dimensions along paths 1-2-3-10-11 and 5-2-12 can be extracted from Figures 4,5 and 6 and compared with measured values as documented in Table 4. These same dimensions assuming a fusion zone temperature of 1400 C are also included in Table 4.

TABLE 4

COMPARISON OF COMPUTED AND MEASURED HAZ WIDTH DIMENSIONS

PATH	FZ BDY TEMP (C)	DISTANCE (mm)		
		FEM	ION	MEASURED
1-2-3-10-11	1450	5.2	4.8	5
	1400	5	4.7	5
5-2-12	1450	4	4.8	3.8
	1400	3.8	4.7	3.8

Notes

- (1) FEM dimensions taken from Figures 4 and 5
- (2) Ion dimensions taken from Figure 6



Figure 7 Nodal values of the retention time above 1000 C for a 3kJ/mm weld.

It is evident that there is reasonable agreement which lends some credibility to the computations.

The retention time above 1000 C is also said to be an important parameter in rationalizing the grain structure encountered in the bay region. The computed nodal distribution is shown in Figure 7. It seems that the retention time above 1000 C is about 10s along the fusion zone boundary. It is about 8s for a mid-bay node but then falls very quickly to 0 beyond this point as would be expected. The validity of these computations is difficult to assess in the absence of measured values for these particular welds. Kohno and Jones [7] find values ranging from 2 to 11.3 seconds in the bay region for similar 3kJ/mm welds. Based on the Kohno/Jones measurements the computations would seem to be high. However, the measurements are difficult to make and there is considerable uncertainty. Therefore, it is not possible to be definitive at this point.

(C) DISCUSSION OF "BAY" THERMAL MODELLING

While there is no doubt that the compound ellipsoid heat source advances weld process modelling, considerable development is still required to guarantee confidence in the computations. As it now stands, selecting the dimensions of two ellipsoids and a power sharing between them is overly complex. There are too many possibilities and the significance of each change is not yet understood. However, the results presented in this report are encouraging. The results demonstrate that a bay configuration is possible with an appropriate choice of parameters. In addition, the computed values seem reasonable and to agree (within reasonable limits) with measurements.

However, recent experiments at the Welding Institute by Barlow [1] would suggest that the fusion zone of a deep penetration submerged arc weld can be considered to be formed by a two stage solidification process. In fact Barlow suggests that the molten pool can be considered as two pools -- a small zone directly beneath the arc that solidifies first and a large capping pool where the solidification is delayed. Apparently the weld pool directly below the arc is depressed and molten metal is forced up behind the heat source. As the arc passes molten metal fills the cavity. Solidification begins at the bottom of the cavity and moves upward. At the same time the large mass of molten metal behind the arc melts out beyond the cavity walls and forms the broad top typical of deep penetration welds. However, solidification of this metal is significantly delayed; to the point that Barlow considers the two events (solidification of the lower and of the upper pools) to be almost separate events.

Metallographic evidence in support for this mechanism is provided by Barlow. He claims a solidification line separating the upper and lower pools. Such a line is evident in the 350WT (CAB) weld shown in Figure 3. This may seem to be superficial perhaps, because the grain structure appears to carry through the line. However, a detailed investigation of this area confirms that it

is more than superficial. In fact the grain continuity must be epitaxial growth which is a well known weld solidification phenomena. It is this authors contention that the solidification line observation in this investigation lends support to the Barlow contention.

Barlow's observations support the concept of modelling deep penetration welds with compound double ellipsoids. However, they also suggest that the upper ellipsoid should be offset (ride behind) the lower ellipsoid. This probably explains why it is so difficult to arrange tandem ellipsoids (one over the other) to form a bay configuration. Beyond this contract the concept of offset ellipsoids should be further developed to provide flexibility in obtaining reliable deep penetration profiles.

HAZ HARDNESS COMPUTATIONS AND MEASUREMENTS

In the early part of the contract period the HAZ hardness levels of the four CANMET off-shore steels were examined and reported. In addition the software was made available to CANMET and a manual was submitted as a contribution to the program. The manual is contained in Appendix B along with the HAZ hardness computations. The results extended below.

There are several methods available in the literature for computing HAZ hardness. Seven relatively independent models are contained in the Carleton computational system. It is shown (Appendix B) that there is considerable consistency among these models, which lends confidence to the hardness values computed. On the other hand it seems that one or two of the models often yields spurious results. In this case (CANMET off-shore steels) the Cottrell model results are high while the Beckert model results are low. Because of the consistency of the other five model results it is reasonable to ignore the Cottrell and Beckert models in this case. It should be noted, however, that ignoring these two models may not always be appropriate. In other welding situations evidence shows that it may be other models that yield spurious results. Nevertheless with some judgment it is almost always possible to arrive at a reliable HAZ hardness value. In addition, there seems to be quite reasonable agreement between computed and measured hardness values for the CANMET steels as shown in Table 5 which lends considerable confidence in the system.

Beyond predicting the HAZ hardness for any given welding situation, the system can also be used for parametric studies such as those shown in Appendix B. There are many situations in practice where a welding engineer wishes to know how the HAZ hardness changes with current, welding speed, etc. At the same time parametric comparative values are inherently more accurate than absolute calculations since many of the model assumptions and approximations cancel i.e. the same assumptions and approximations apply to all calculations and therefore cancel (more or less) when comparative values are examined. By comparing the response of the 350WT (CAB) to that of the 350WT (STRAND) it

is clear that current and carbon content have considerable effect on the HAZ hardness of these steels. On the other hand preheat temperature surprisingly has relatively little effect.

TABLE 5

HAZ HARDNESS LEVELS FOR THE CANMET OFF-SHORE STEEL WELDS

Material	Measured Hardness VPN	Computed Hardness VPN
350WT (CAB)	264	258
BS4360	236	232
LT60	240	244
350WT (STRAND)	216	218

Notes

- (1) The measured values are a mean of 25 measurements from five location (2 near surface locations; 2 bay locations and a root location).
- (2) These are microhardness measurements adjacent to the weld metal using a 500g weight -- see Figure 8
- (3) The computed values consisted of an average of the results of 5 models (Arata, Yurioka, Suzuki, Teresaki and Dueren)
- (4) Cooling time - 20s

While such models are quite useful in practice, they provide only a single HAZ hardness value unless combined with FEM computations. It is the contention of this investigator that a single computed HAZ value is not a problem because hardness varies slowly with cooling time and cooling time differences around the periphery of a weld are not large. On the other hand grain growth in the bay could increase the hardenability which, in turn, should have some effect on the hardness in this region. Hardnesses measured and computed using FEM cooling times at various locations around the periphery of the 350WT (CAB) weld are contained in Table 6. It seems clear from these measurements that a single computed hardness value is sufficient at least for this welding situation.

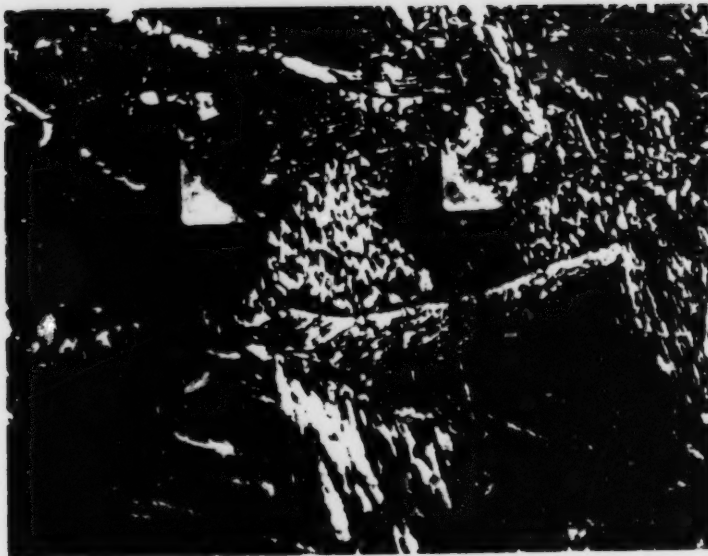


Figure 8 Microhardness indentation in the HAZ at the weld line.

TABLE 6**MEASURED AND COMPUTED HAZ PERIPHERY HARDNESS VALUES**

Position	Cooling Time 800/500 C (s)	Measured Hardness VPN	Computed Hardness VPN
Surface	16.6	270	274
Bay	19.1	268	256
Root	19.6	252	257

Notes (1) Measurements are an average of five readings with microhardness (500g) weight - see Figure 8

(2) Calculated values obtained by taking cooling times from FEM computations and submitting these to the hardness software

It is also interesting to note that point source computations provide a cooling time of 16s in this case which corresponds to a hardness of 272 VPN. This is reasonably close to the more accurate value obtained as a result of applying FEM computed cooling times. However, it should be noted that point source cooling times are slightly less than measured and FEM values. Therefore, hardness values computed with point source cooling are likely to be slightly high. With some allowance, it is this authors view that hardness can be computed using cooling times calculated with conventional point source models for most purposes.

PREHEAT COMPUTATIONS

Software based on the Nippon Steel method for calculating the preheat level necessary to prevent cold cracking was also submitted to CANMET as part of the early contribution to this contract. However, the software is relatively uninteresting with respect to the four CANMET welds because it indicates that no preheat is necessary. This might be expected since a 3kJ/mm weld is a relatively high heat input and the CANMET steels are low carbon equivalent materials.

Preheat computations are contained in Appendix B for SMA field welds (350 (CAB) and 350 (STRAND) materials). Once again the flexibility and value of such software for parametric studies is demonstrated. The results would indicate that in general SMA welding requires preheat to prevent cold cracking in the HAZ. Figures generated with the software are shown to point out the relative importance of carbon level and joint preparation. On the other hand current level and even hydrogen level do not seem to

have a large effect on preheat. Interestingly enough ambient temperature has a considerable effect on the preheat level of the 350WT (CAB) material but little effect on the preheat level of the 350WT (STRAND) material.

MICROSTRUCTURE COMPUTATIONS

Microstructure distributions in the HAZ can be computed according to the algorithm suggested by Watt et al [10] and enhanced by Bibby et al [11]. Recent papers that describe the algorithm in detail are contained in Appendix C. The most sensitive area of the HAZ is the region immediately adjacent to the weld metal. The computed HAZ microstructures along the weld line for the CANMET welds are contained in Table 7.

TABLE 7

COMPUTED HAZ WELD LINE MICROSTRUCTURES

Material	Fraction Martensite	Fraction Bainite
350WT (CAB)	0.29	0.71
BS4360	0.23	0.77
LT60	0.22	0.78
350WT (STRAND)	0.20	0.80

Notes

Cooling time - 20s

Heat Input - 3kJ/mm

The results of these computations suggest a level of martensite that is surprisingly high [9]. At this point, however, there are no measured results to assess the validity of the calculations. In view of this the accuracy remains an open question.

It is also surprising to find that the calculated martensite level of the 350WT (CAB) material with a carbon content of 0.15w/o is 29% while that of the 350WT (STRAND) material with a carbon content of 0.07w/o is 20%. This investigator would have expected a larger difference and perhaps much less martensite in the low carbon material.

It is not clear to what the difficulty might be attributed, if indeed there is a difficulty. The answer to this lies beyond the scope of this contract.

ADDITION OF FUSION ZONE MICROSTRUCTURE ALGORITHM

Discussion of the HAZ microstructure algorithm in the last section was brief because a detailed version can be found in Appendix C. This, however, should not be interpreted as an indication that microstructure computations are not important. Quite the contrary - predicting HAZ microstructures it is very important.

Similarly a microstructure computational system for the weld metal is equally important. Yet it has always been considered a very difficult problem because of the complexity of structure formation in this region. However, it seems that Bhadeshia and Associates [6] at Cambridge University have succeeded in establishing such an algorithm. The secret seems to be in judicious approximations to solidification theory and in recognizing diffusional rate limiting conditions where appropriate. While it is beyond the scope of this contract, it is nevertheless important to call attention to this work and suggest further work in this area.

PAPERS AND PRESENTATIONS ARISING FROM THIS CONTRACT

The contract began in November 1985. Since that time four papers were published and four were presented as a result of the work. The published papers are contained in Appendix C together with abstracts of the presentations.

ACKNOWLEDGMENTS

My thanks to Dr. John Bowker (CANMET) for encouraging and collaborating in this work. Thanks also to Dr. Jim McGrath for his support. I would also like to acknowledge the contribution of Dr. John Goldak and Mr. Warren Hik for the compound ellipsoid analysis.

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APPENDIX A

Documented in this Appendix are the measured cross-sectional dimensions of the CANMET off-shore steel welds, and the computed melting temperatures and eutectoid temperatures for these steels.

TABLE 8

CROSS-SECTIONAL DIMENSIONS OF THE CANMET WELDS

Steel	C (w/o)	Penetration (mm)			Width (mm)		FZ-HAZ	
		Reinf	FZ	HAZ	Surface	Bay	S1	S2
350WT (STRAND)	0.07	15	10.5	12	18	11	3.1	4.15
LT60	0.12	15	11	12.5	18.5	12	3.8	3.1
BS4360	0.14	16	11.5	13.5	19.5	13	4	3.2
350WT (CAB)	0.15	15	11.5	13.5	20	13.5	4	4

Notes

(1) Penetration

Reinf: distance from the top of the reinforcement to the root tip

FZ : distance from the surface to the root tip

HAZ : distance from the surface to the HAZ root tip

(2) Width

FZ : width of the fusion zone at the surface

Bay : width of the fusion zone at the top of the bay

(3) FZ-HAZ

S1 : width of the HAZ perpendicular to the lower side of the bay (side 1) -- at the top of the bay

S2 : width of the HAZ perpendicular to the lower side of the bay (side 2) -- at the top of the bay

TABLE 9

MELTING POINT AND EUTECTOID COMPUTATIONS FOR THE CANMET STEELS

Material	Melting Temp (C)	Eutectoid Temp (C)
350WT (STRAND)	1530	716
LT60	1526	717
BS4360	1524	719
350WT (CAB)	1523	710

Notes:

(1) Formulations taken from the work of Ion et al (reference 4)

$T_m = 1810 - 90(w/o C)$ degrees K

$A_E = 996 - 10.7(Mn) - 16.9(Ni) + 29.1(Si) + 16.9(Cr) + 290(As) + 6.38(W)$ degrees K

APPENDIX B

Contained in Appendix B is a copy of the mid-contract report prepared to describe software for computing HAZ hardness and preheat temperature to avoid cold cracking.

WELD QUALITY SOFTWARE FOR THE MS-DOS COMPUTERS

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January 1987

WELD QUALITY SOFTWARE FOR THE HP71B HAND HELD COMPUTER

Summary

The following is an "operations procedure" manual for two weld quality software programs implemented on a PC (personal computer) with an MS-DOS operating system. The two software models are:

(1) Adams: A software system for predicting the HAZ (heat-affected zone) and WZ (weld zone) hardness given the input welding parameters (voltage, current, welding speed, process efficiency, and preheat temperature), and the chemical composition of either the base material HAZ or WZ whichever is relevant. Note that the weld zone composition can be estimated from the compositions of the base metal and filler assuming a realistic process dilution. The results appear as hardness (VPN) values computed using the Adams transition cooling theory (Ref. 1) and the hardness + composition models according to:

- | | |
|----------------|-----------|
| (1) Arata | (Ref. 2) |
| (2) Yurioka I | (Ref. 3) |
| (3) Suzuki | (Ref. 4) |
| (4) Cottrell | (Ref. 5) |
| (5) Teresaksi | (Ref. 6) |
| (6) Beckett | (Ref. 7) |
| (7) Dueren | (Ref. 8) |
| (8) Yurioka II | (Ref. 14) |

In addition to computed hardness values, fraction martensite is calculated using the Arata and Yurioka II models. It should be noted that the Yurioka II model applies primarily to reasonably rich quench and tempered materials (e.g., the HY series) whereas all other models apply primarily to microalloy and low alloy structural steels. The references should be consulted for precise compositional ranges.

Since predicting weld hardness and fraction martensite is a semi-empirical business, several models are contained in the software to provide a relatively wide basis for judgement in practice. Experience suggests that the Cottrell model is often high and the Beckett model is often low. Values computed for some low carbon off-shore steels are attached to this manual to demonstrate this point.

(2) Preheat: A software system for calculating the preheat necessary to avoid hydrogen cracking - based on the theory put forward by Nippon Steel Researchers - primarily Yurioka (Ref. 10). The input consists of the welding parameters, workpiece size, joint shape, process hydrogen level (IIW), restraint level, yield strength, and chemical composition. If local preheat is involved, the width of the heated zone and preheater intensity must also be submitted to the computer.

Step-By-Step Procedure

- (1) Turn the PC system on and load the DOS operating system in the usual way.
- (2) To run either program type
> [Name of Program]
e.g. ADAMS
e.g. PREHEAT
- (3) From this point on all you do is answer the questions (prompts) that appear on the screen. Example computations are shown in Tables 1 and 2.

Table 1

STEP-BY-STEP PROCEDURE FOR RUNNING THE ADAMS SOFTWARE

STEP	INSTRUCTIONS	DISPLAY	INPUT
P			
1	Run Program		ADAMS
2	Enter Composition	%C=	0.15
3		%MN=	1.08
4		%SI=	0.20
5		%NI=	0.28
6		%CR=	0.30
7		%MO=	0.05
8		%V=	0.02
9		%B=	0
10		%CU=	.02
11		%NB=	.01
12		%N=	.008
13		%S=	.01
		DATA OK Y/N	Y
14	Program checks the steel type:		
	HT TYPE STEEL		
15		COOLING TIME (sec) or (0)	[Note 1]
16	Input Welding Parameters:	Voltage =	25
17		Amps =	350
18		ARC EFFY =	.95
19		ROOM TEMP (celcius) =	20
20		THICKNESS/DEPTH (mm) =	38.1
21		WELD SPEED (mm/s) =	5
22	Program checks type of heat flow	3D HEAT FLOW	
23	ADAMS COOLING TIME =	8.5 sec	
24	ARATA HARDNESS (VPN) =	315.4	
25	FRACTION MARTENSITE (ARATA) =	0.574	
26	YURIOKA HARDNESS (VPN) =	336.3	
27	COTTRELL HARDNESS (VPN)	339.9	
28	SUZUKI HARDNESS (VPN) =	302.1	
29	TERASAKI HARDNESS (VPN) =	302.6	

30 BECKERT HARDNESS (VPN) = 257.4
31 DUEREN HARDNESS (VPN) = 329.8
32 YURIOKA II HARDNESS (VPN) = 304.12
33 FRACTION MARTENSITE (YURIOKA II) = 0.445
34 DO YOU WISH TO CALCULATE ANOTHER COOLING TIME ? (Y/N) N

[Note 1] When the program requests COOLING TIME (sec) or 0, a 0 does not mean a cooling time (800 to 500 C) of 0, but is simply a means of passing to the next step (voltage, current, etc.) If the cooling time is known, i.e., measured experimentally or if you wish to put in values to see how the hardness responds, then insert cooling time instead of 0 and the program skips straight to the hardness output.

STEP-BY-STEP PROCEDURE FOR RUNNING THE PREHEAT SOFTWARE

STEP	INSTRUCTIONS	DISPLAY	INPUT
1	Run Program	** Program PREHEAT **	PREHEAT
2	Enter Composition	Input COMPOSITION	
3		%C=	0.21
4		%SI=	0.20
5		%Mn=	1.08
6		%Cu=	0
7		%Ni=	0.28
8		%Cr=	0.30
9		%Mo=	0.06
10		%V=	0.02
11		%Nb=	0
		%B=	0
	Output	CARBON EQUIVALENT, CE _{Yur} =0.485	
12	Check Composition Data	DATA OK (Y/N)	Y
13	Enter Values	Input WELDING CONDITIONS	
14		EFFY=	.95
15		VOLTS=	25
16		AMPS=	350
		WELD SPEED (mm/s)	5
	Output	Energy Input, EJ(J/mm)=	1750.0
17	Enter Method	HYDROGEN Method, HJIS/HIIW:? HIIW	
18	Enter Value	HIIW (ml/100gr):?	15
19	Enter Values	Input RESTRAINT CONDITIONS:	
20		PLATE THICKNESS, h(mm):?	38.1
21		rf, (N/mm ³):?	400
22		Y.S., y (N/mm ²):?	400
23		S.C.F., Kt:?	1.5
	Check Welding Data	Welding data OK (Y/N)	
	Output	Cr. COOLING TIME (s) =	1764.6
24		AMBIENT TEMPERATURE, T(C):?	20
25	Select Preheat Method	PREHEAT METHOD - Uniform or local ?	U
26	Enter Values	LENGTH, L(mm)=?	4000
27		WIDTH, W(mm)=?	400
28	Output	MINIMUM PREHEAT TEMP., T _{ph} (C)=102.5	
29	Select Program Options	Run again, View again, or End ? (R\V\E)	R

```

      If R then repeat
      steps 13 to 25
30    Select Preheat
      Method
31    Enter Values
      PREHEAT METHOD - Uniform
      or Local? (U/L) L
32    WIDTH of Preheat Zone, 2B(mm):? 100
      H.D. of Heater, q(J/mm2.s):? 0.084 [Note 1]
      Computing . . .
33    Output
      PREHEAT TIME, tph(s)=2385.4
34    Min. PREHEAT TEMP., Tph(C)=155.4
35    Select Program
      Run again, View again, or End?R E
      Options

```

[Note 1] Local preheat assumes an electrical strip heater of width "2B". The heating density (H.D.) is the linear heat input rate of the heater (J/m.s) divided by the thickness of the workpiece section.

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APPENDIX A

Heat-Affect Zone Hardness and Preheat Computations For the 3kJ/mm EMR Off-Shore Steel Welds

Computations: Table 1

Steel Compositions: Table 2

CONCLUSIONS

- 1) Of the seven methods available for computing HAZ hardness, values calculated with the Cottrell method are consistently high while values calculated with the Beckert method are consistently low.
- 2) Values calculated with the Arata, Yurioka, Suzuki, Teresaki and Dueren methods are consistent and within a few hardness points for all four steels at the 3 kJ/mm level.
- 3) The Adams and Kohira cooling times (15.8 and 16.1 s respectively) are somewhat lower than the FEM values (16.6 to 19.6 - position dependent) and the experimental value of 20 s. This will have some effect on the HAZ hardness computed.

Note: there is theoretical justification for adjusting the Adams/Kohira values upward by $\approx 20\%$. This corresponds to changing the mean conductivity from 25 to 21 J/(m°C s) which is a matter of debate in the literature. By making this change the cooling times and HAZ hardness computations would be consistent among the cooling models.

TABLE 1

HARDNESS AND PREHEAT COMPUTATIONS

FOR THE 3kJ/mm EMR OFF-SHORE

STEEL WELDS

	<u>LT60</u>	<u>BS4360</u>	<u>350WT(STRAND)</u>	<u>350WT(CAB)</u>
<u>Cooling Time: 15.8(s)</u> (ADAMS)				
Hardness				
Arata	253	243.0	222.5	273.0
Yurioka	262.5	246.3	230.0	278.8
Cottrell	296.4	276.3	354.0	299.2
Suzuki	256.0	246.6	219.2	266.6
Teresaki	257.2	247.9	230.8	280.9
Beckert	221	209.4	207.6	227.0
Dueren	257.8	242.4	230.9	272.3
<u>Cooling Time: 16.06</u> (KOHIRA)				
Arata	252.5	242.4	222.1	272.2
Yurioka	263	245.3	229.3	277.6
Suzuki	255.2	245.7	218.6	265.4
Cottrell	295.4	275.1	352.6	298.1
<u>Cooling Time (FEM): 20s</u> (16.6 to 19.6)				
Arata	244.4	234.6	216.6	262.2
Yurioka	247.9	233.5	220.4	262.1
Cottrell	279.5	257.9	333.4	282.2
Suzuki	243.9	234.8	211.3	252.1
Teresaki	242.2	233.7	221.6	260.9
Beckert	213.2	202.2	202.4	217.6
Dueren	240.1	222.5	218.2	251.4
<u>Preheat (Uniform)</u>				
	No preheat needed	No preheat needed	No preheat needed	No preheat needed

TABLE 2

COMPOSITION OF THE EMR OFF-SHORE STEELS

<u>STEEL</u>	<u>C</u>	<u>Mn</u>	<u>Si</u>	<u>Cr</u>	<u>Ni</u>	<u>Mo</u>	<u>V</u>	<u>Cu</u>	<u>Nb</u>	<u>S</u>	<u>N</u>	<u>P</u>	<u>Al</u>	<u>Sn</u>	<u>Ti</u>
LT60	.12	1.29	.272	.151	.135	.101	.053	.159	.039	.008	.007	.015	.029	.001	-
BS4360	.14	1.33	.370	.015	.010	.010	-	.032	.027	.010	.0073	.020	.030	.001	-
350WT (STRAND)	.07	1.35	.286	.241	.255	.010	.068	.008	.022	.004	.0062	.015	.040	.001	.01
350WT (CAB)	.15	1.44	.240	.040	.225	-	.060	.015	.020	.005	-	.015	.015	<.005	<0.01

APPENDIX B

Effects of Welding, Workpiece and Environmental Variables on the Hardness and Preheat Levels for 350 (STRAND) and 350 (CAB) PMRL Experimental Steels.

- Figure 1: Hardness vs current
2: vs preheat level
3: Preheat temperature vs current
4: vs stress concentration
5: vs hydrogen level
6: vs ambient temperature

CONCLUSIONS

- 1) On average the HAZ hardness of the STRAND material is some 75 VPN points less than the CAB material under the same welding conditions.
- 2) Preheat has a relatively small effect on HAZ hardness (20 VPN points for -25 to 100°C preheat range) whereas welding current i.e. heat input has a relatively large effect (130 VPN points for a range of 100 to 800 amps)
- 3) As expected the preheat level required for the STRAND material is considerably less than it is for the CAB material ($\approx 100^\circ\text{C}$ on average).
- 4) Preheat will always be needed for low current (< 400 amps i.e. < 1.5 kJ/mm) welding with the (CAB) material but under favorable conditions ($T_o > 20^\circ\text{C}$, $K_t < 2$, HIIW < 25 ml/100g, restraint $r_f < 400$ N/mm², yield level < 500 mPa). preheat will not be needed for the STRAND material.
- 5) The large effect of joint preparation i.e. K_t (stress concentration) on preheat value should be noted.

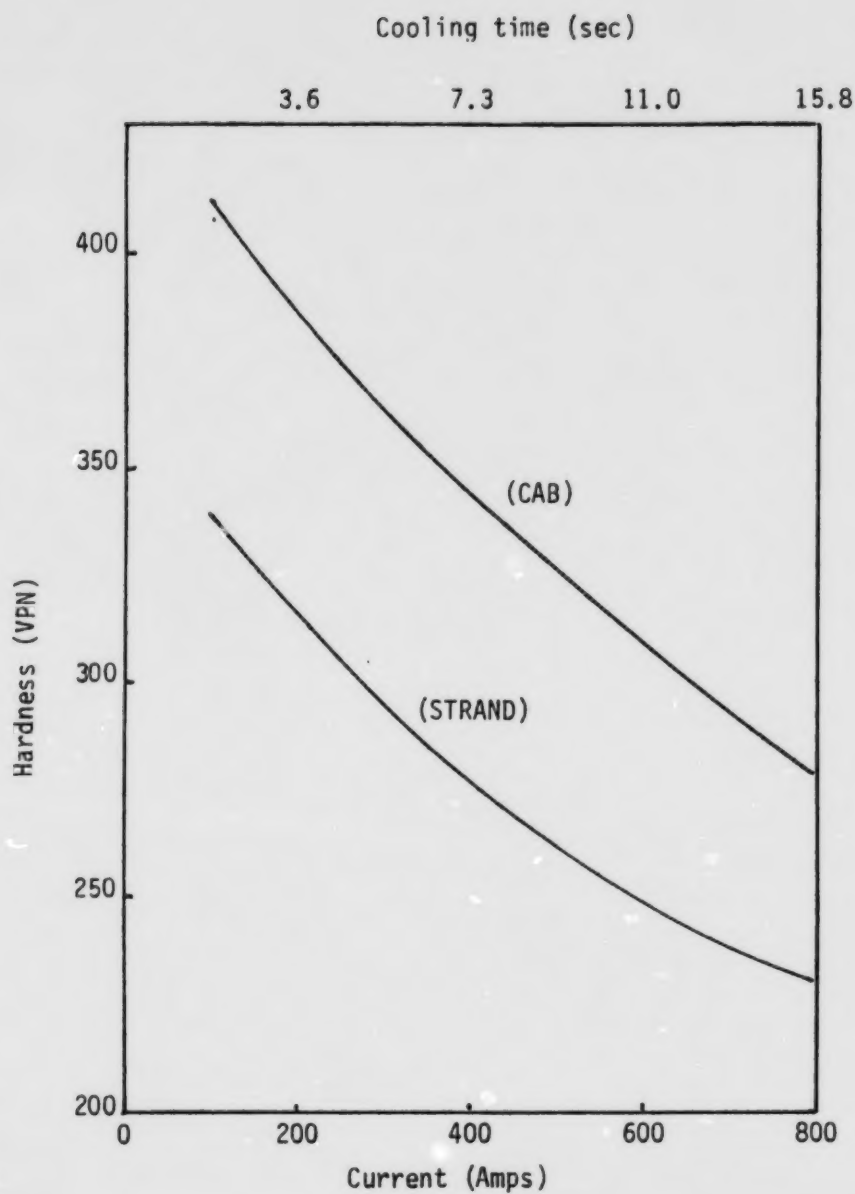


Figure 1 - Effect of welding current on the hardness of the 350 (STRAND) and 350 (CAB) PMRL experimental steels [welding parameters: voltage - 35 volts, welding speed - 9.33 mm/s, preheat temperature - 20°C; plate thickness - 25 mm].

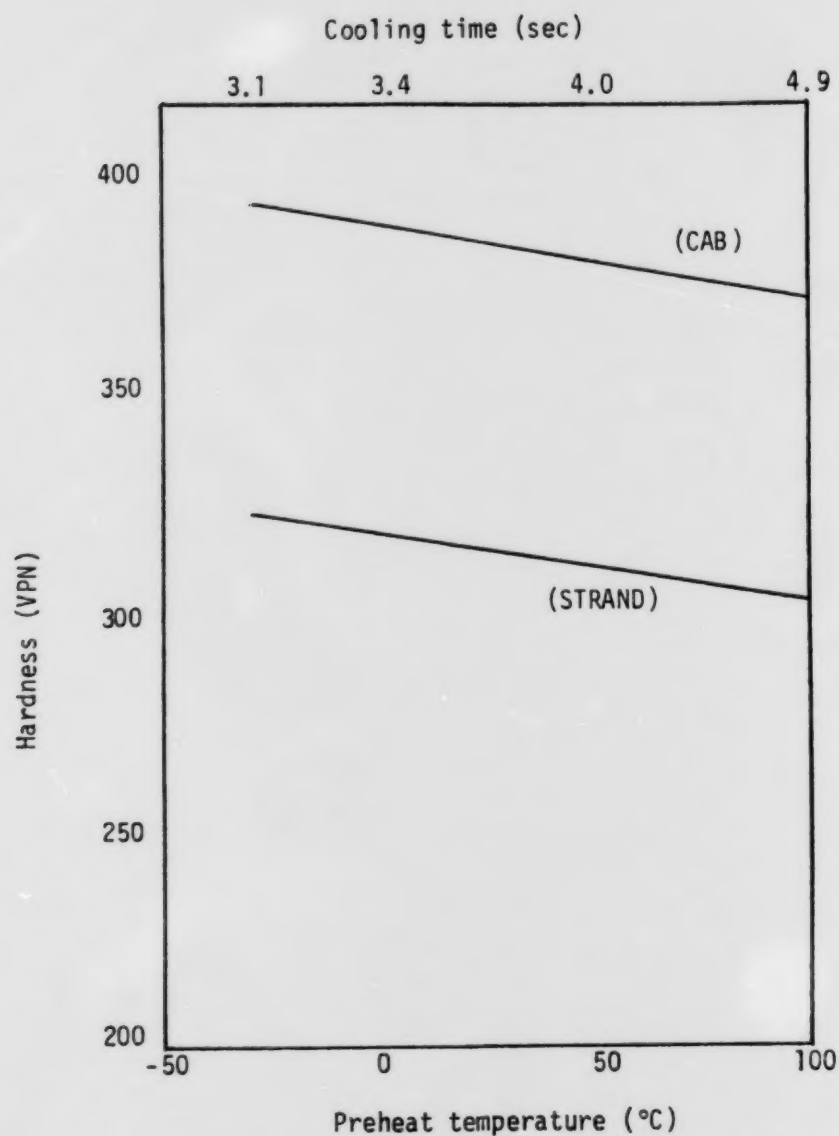


Figure 2 - Effect of preheat temperature on the hardness of the 350 (STRAND) and the 350 (CAB) PMRL experimental steels [welding parameters: voltage - 35 volts, welding current - 200 amps, welding speed - 9.33 mm/s; plate thickness - 25 mm].

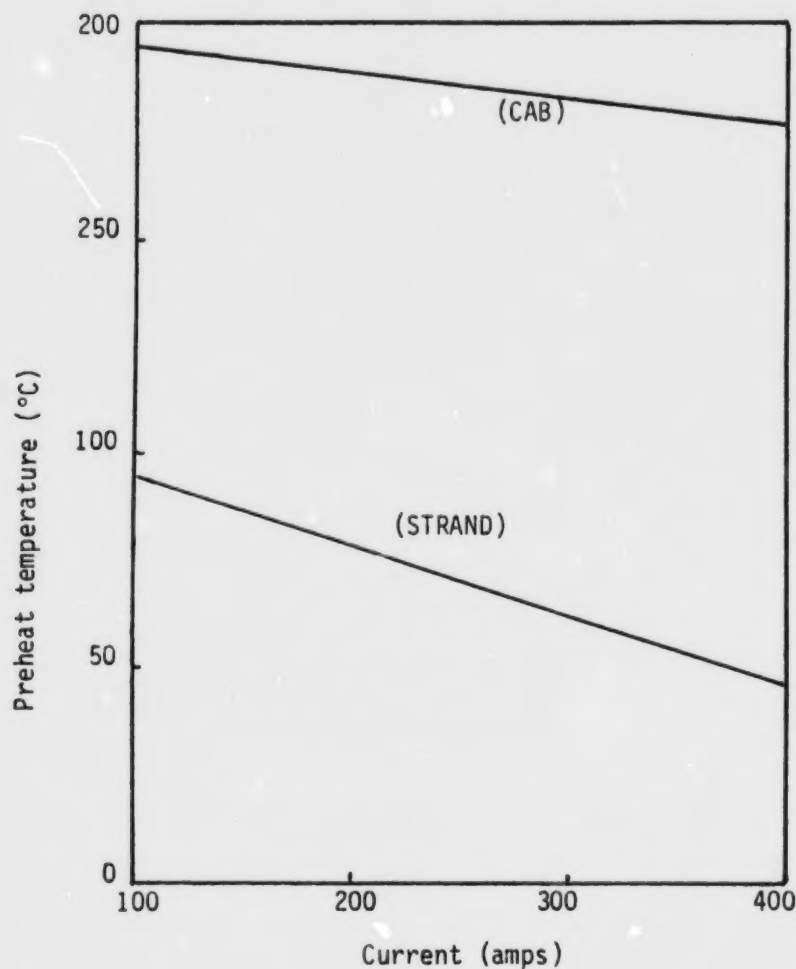


Figure 3 - Effect of current on preheat temperature for the 350 (STRAND) and the 350 (CAB) PMRL experimental steels [welding parameters: voltage - 35, speed - 9.33/mm/s, submerged arc process ($\eta = 0.95$) ambient temperature - 20°C, uniform preheat - plate dimensions - 500 x 350 x 25 mm, stress concentration $K_t = 3.5$, HIIW hydrogen - 25 ml/100 g, restraint - 400 N/mm², yield level - 500 mPa].

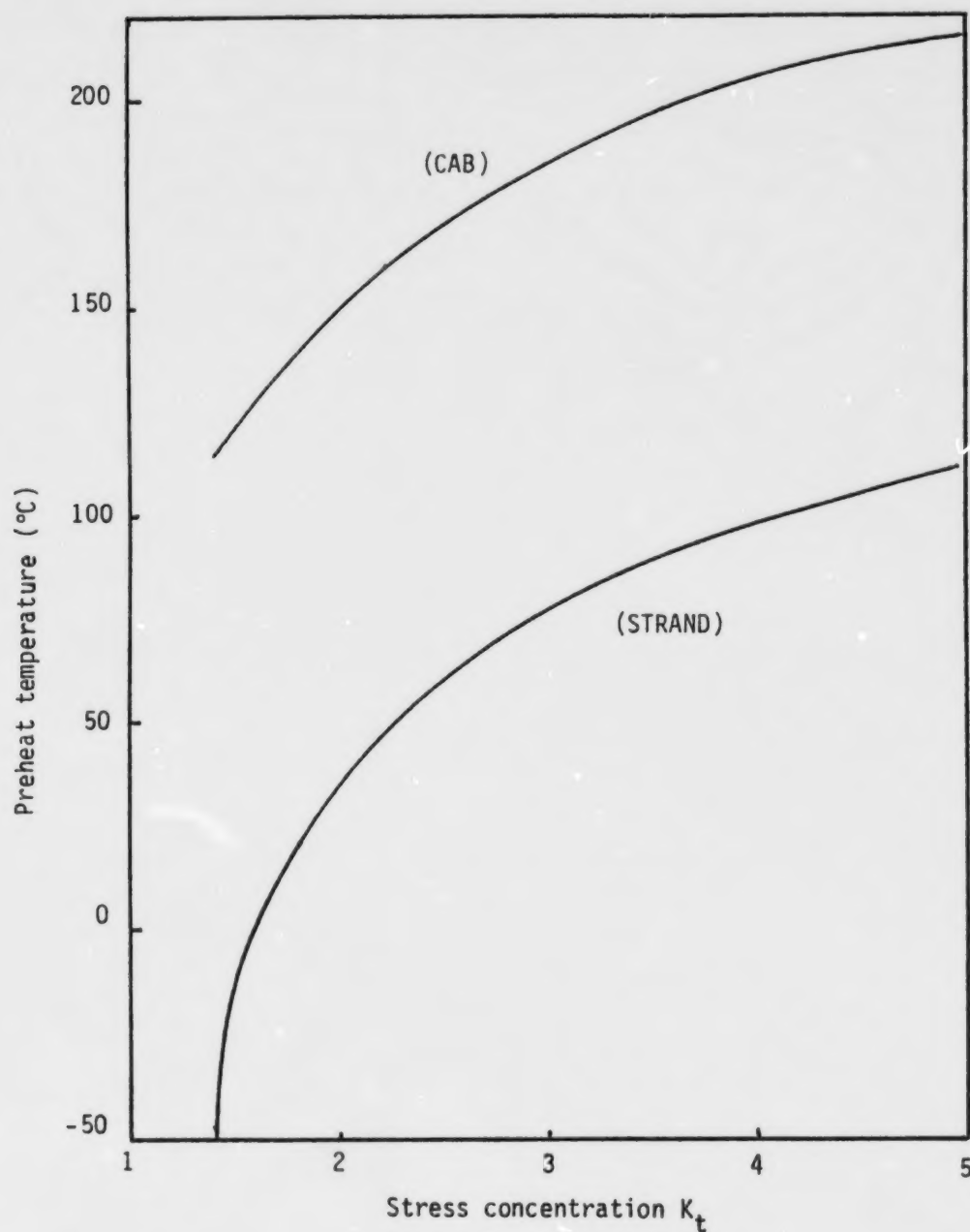


Figure 4 - Effect of stress concentration on the preheat temperature for the 350 (STRAND) and the 350 (CAB) PMRL experimental steels [welding parameters: voltage - 35 volts, weldi speed - 9.33/mm/s, current - 200 amps, submerged arc process ($\eta = 0.95$) ambient temperature - 20°C, uniform preheat, plate dimensions - 500 x 350 x 25 mm, hydrogen level (HIIW) - 25 ml/100 g, restraint - 400 N/mm³, yield level - 500 mPa]

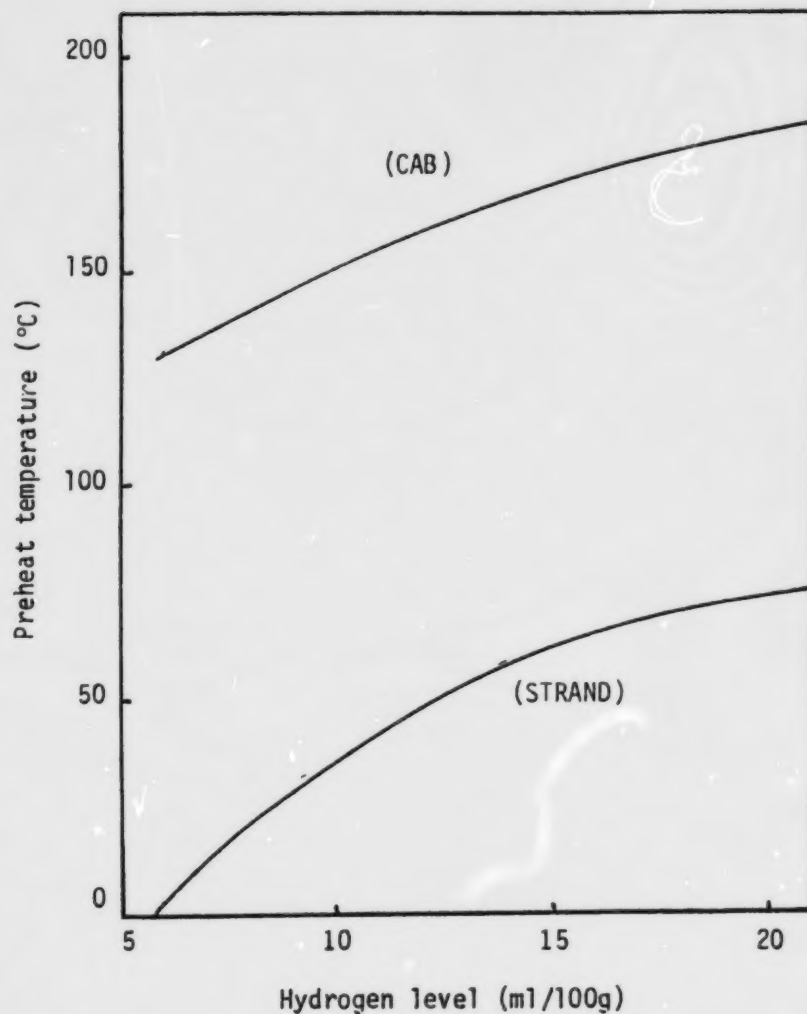


Figure 5 - Effect of hydrogen level (HIIW) on the preheat temperature for the 350 (STRAND) and the 350 (CAB) PMRL experimental steels [welding parameters: voltage - 35 volts, speed - 9.33/mm/s, current - 200 amps submerged arc ($\eta = 0.95$), ambient temperature - 20°C uniform preheat, specimen dimensions - 500 x 350 x 25 mm, restraint level - 400 N/mm³, yield level - 500 mPa, stress concentration - 3.5].

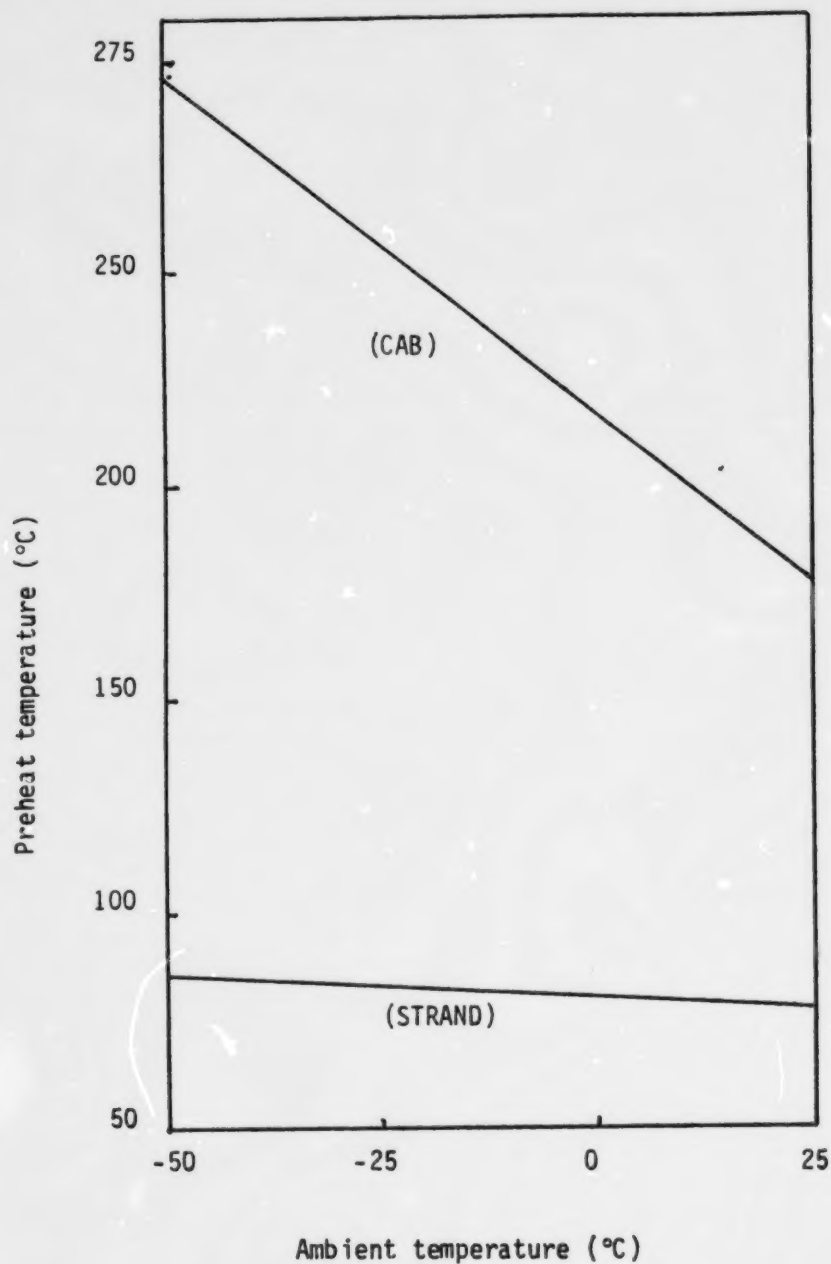
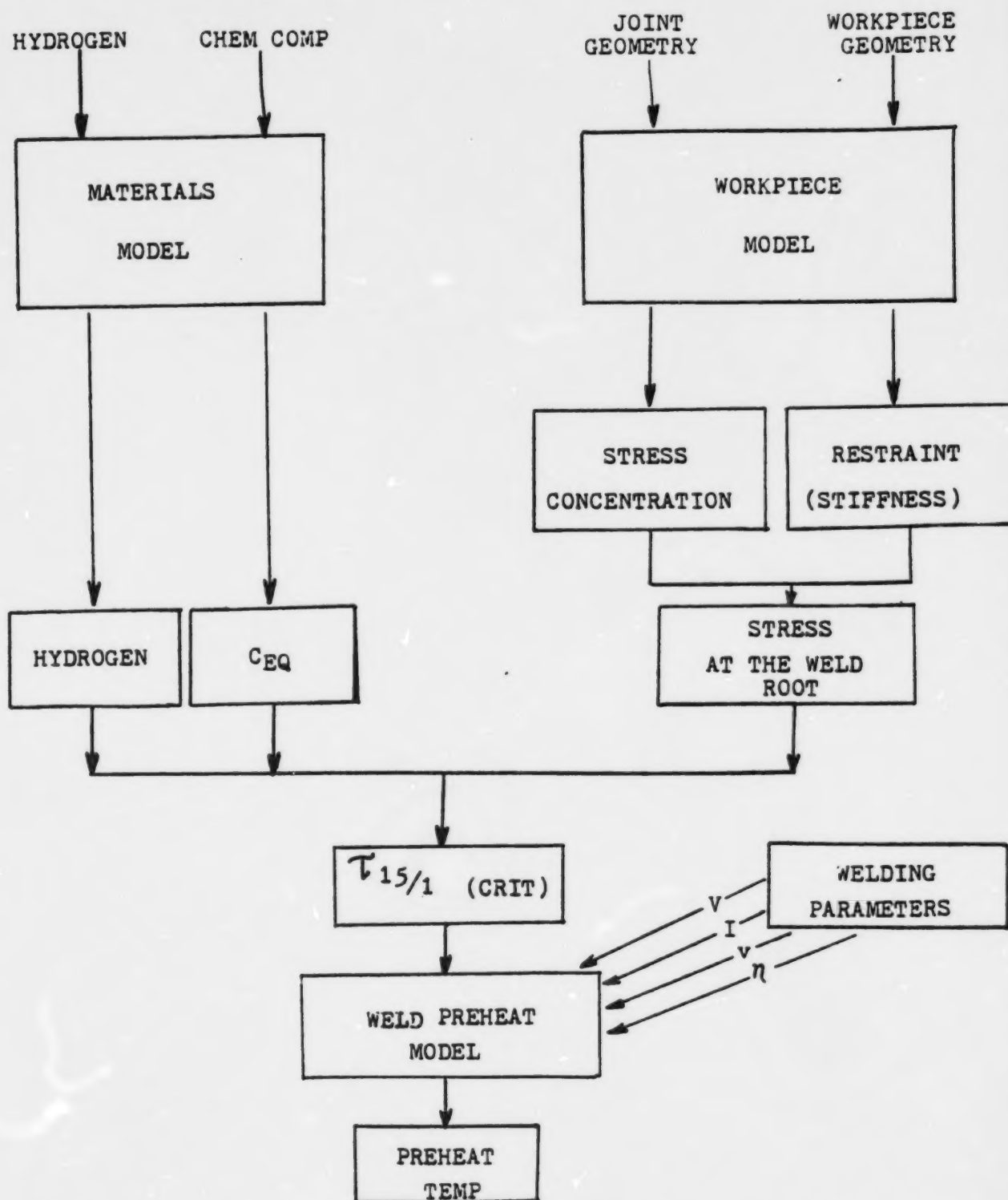


Figure 6 - Effect of ambient temperature on the preheat level for the 350 (STRAND) and the 350 (CAB) PMRL experimental steels [welding parameters: voltage - 35 volts, speed - 9.33 mm/sec, current - 200 amps, submerged arc (η - 0.95) uniform preheat, specimen dimensions - '500 x 350 x 25 mm, restraint - 400 N/mm², yield level - 500 mPa, stress concentration - 3.5, hydrogen level (HIIW) - 25 ml/100 g.]

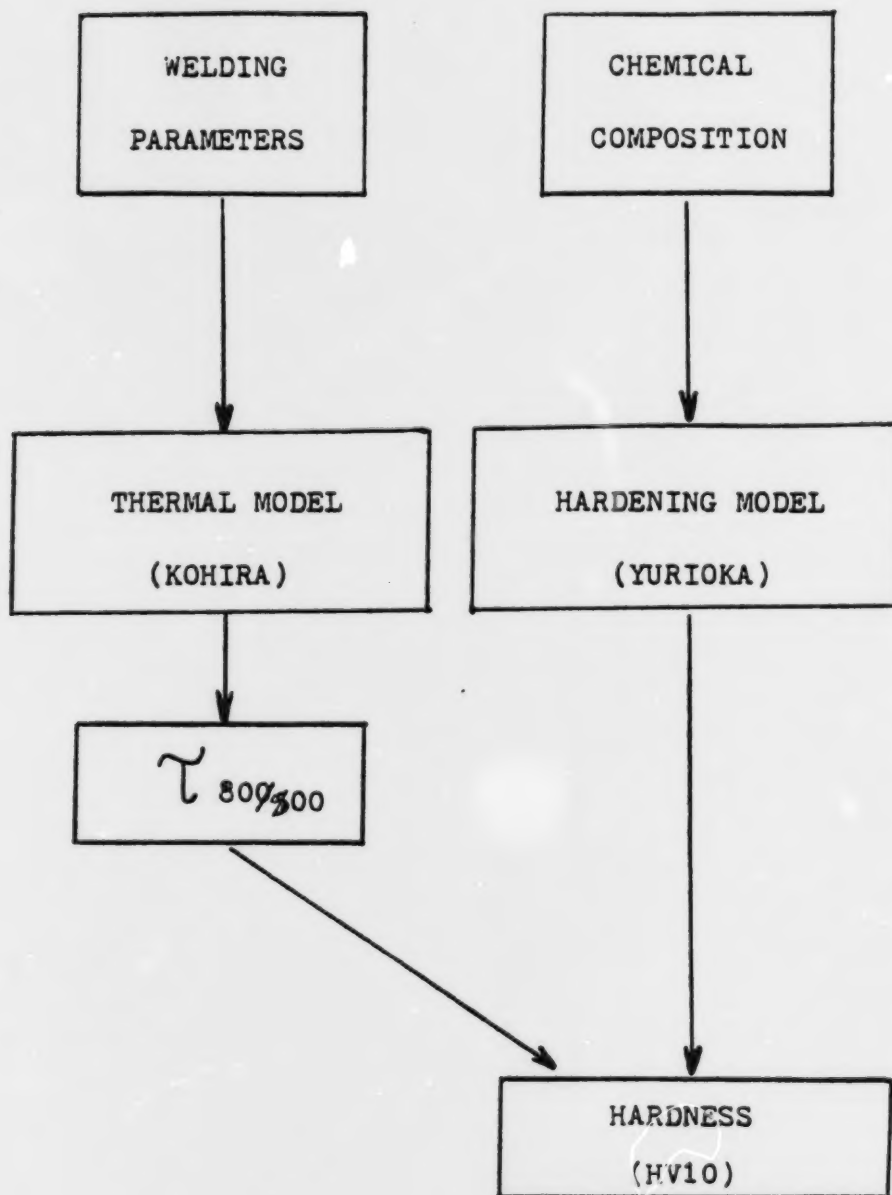
APPENDIX B

Algorithm Flowcharts

Predicting Preheat Levels to Prevent Cold Cracking



Predicting HAZ and WM Hardness



APPENDIX C

Further Information on Preheat Program

APPENDIX C

The following diagrams have been extracted from a number of sources and are useful as input to the PREHEAT algorithm. Since they are routinely used in the preheat computation they are discussed individually below.

(A) Process Efficiency

Weld process efficiencies are subject to considerable measurement error and variation. There is, therefore, considerable debate over the values that should be used. The efficiency values of Figure C1 are suggested based on a review of the literature.

(B) Stress Concentration Factors

Stress concentration based on joint preparation plays a significant role in the formation of HAZ cold cracks. The values suggested by Yurioka [1983] are listed in Figure C2.

(C) Weld Hydrogen Level

The hydrogen level of as deposited weld metal is process dependent. In the absence of hydrogen content measurements the diagram generated by Coe [1975] of the British Welding Institute can be used for estimating the expected level (refer to Figure C3).

FIGURE C1: Suggested Process Efficiencies

Process	Efficiency
SMAW	0.80
SAW	0.95
GMAW	0.75
CO ₂	0.80
GTAW	0.65
EB	0.85

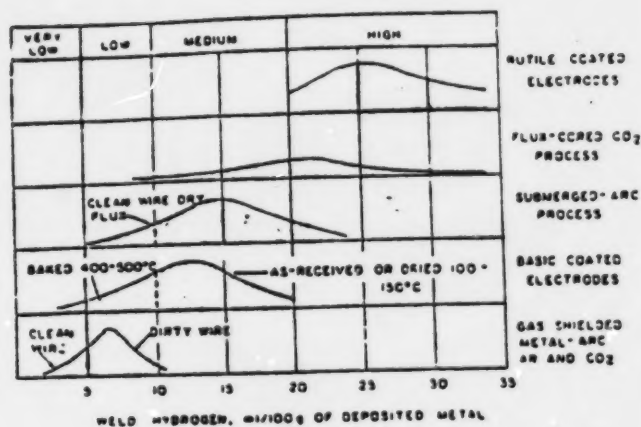


Fig. C 3 Typical hydrogen levels of the deposit metal for various welding processes (after Coe [1975]).

Groove type		K _t
Y (root)		
Double-Vee (root)		3.3
Y (root)		4-5
Single-bevel (root)		5-8
V (root)		1.5
Y, X, Y, V, U (toe)		1.5

Fig. C 2 Stress concentration factors (root or toe) for various weld preparations (after Yurioka

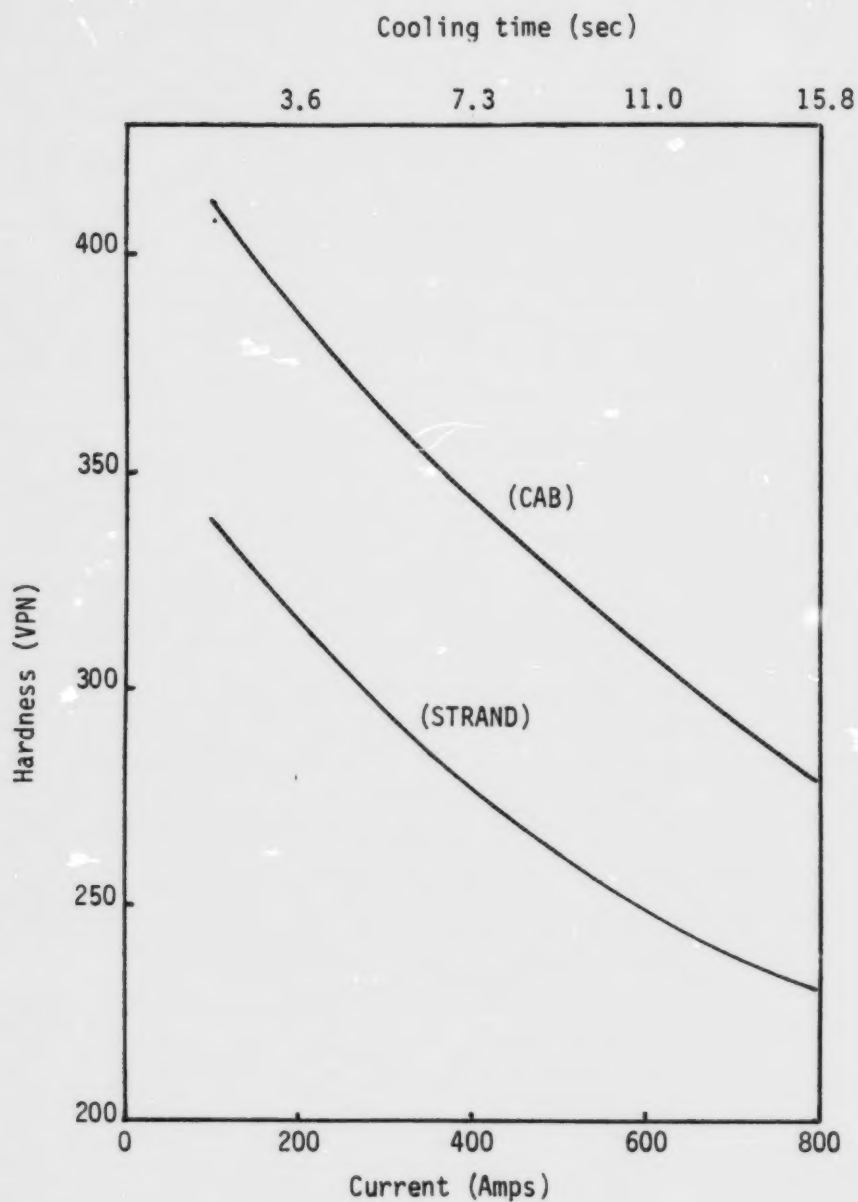


Figure 1 - Effect of welding current on the hardness of the 350 (STRAND) and 350 (CAB) PMRL experimental steels [welding parameters: voltage - 35 volts, welding speed - 9.33 mm/s, preheat temperature - 20°C; plate thickness - 25 mm].

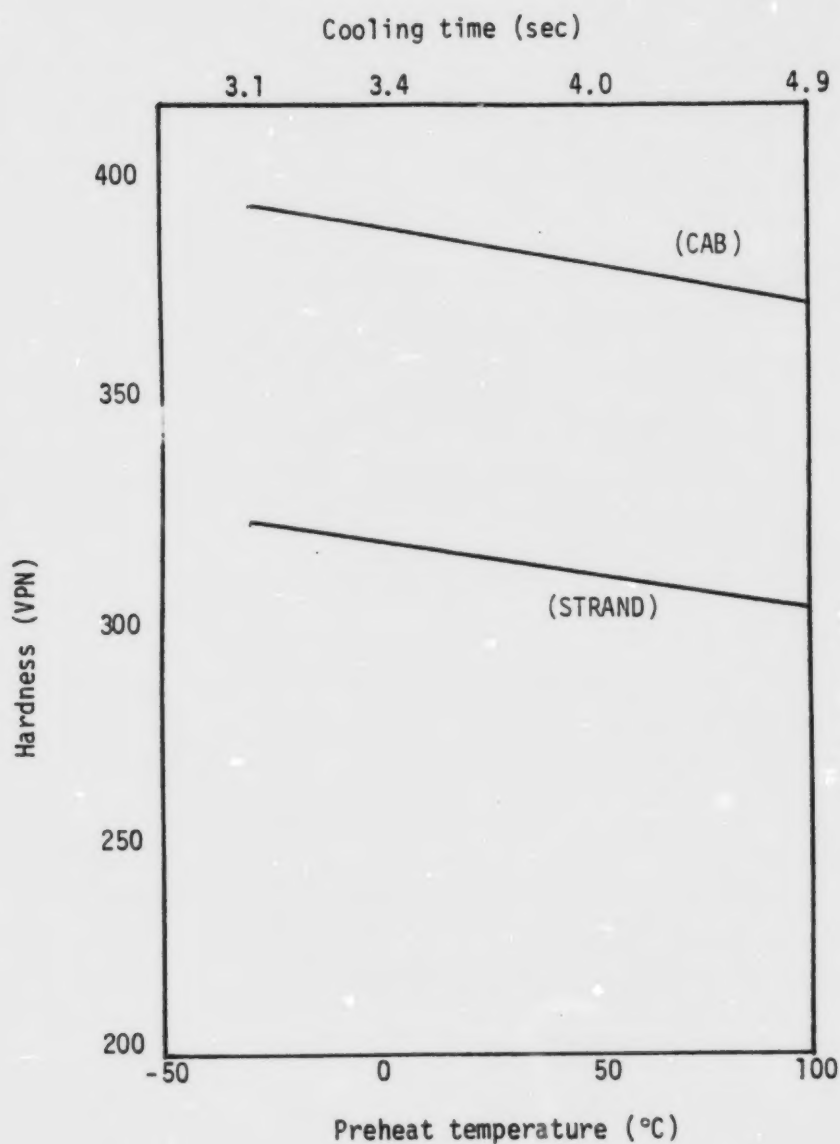


Figure 2 - Effect of preheat temperature on the hardness of the 350 (STRAND) and the 350 (CAB) PMRL experimental steels [welding parameters: voltage - 35 volts, welding current - 200 amps, welding speed - 9.33 mm/s; plate thickness - 25 mm].

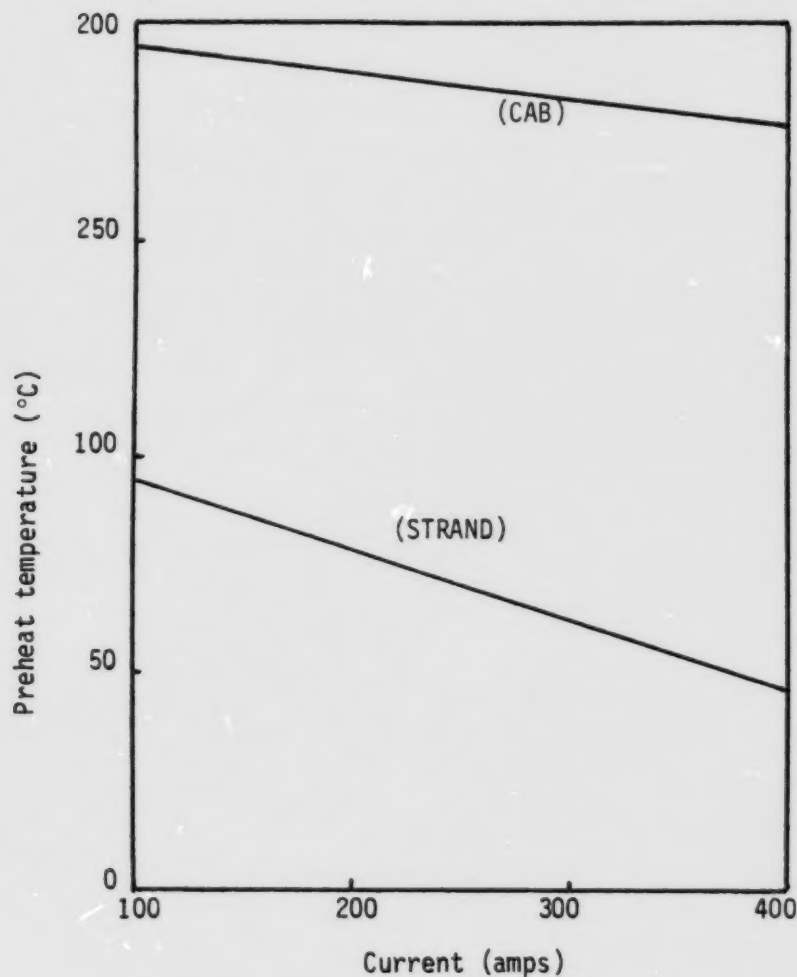


Figure 3 - Effect of current on preheat temperature for the 350 (STRAND) and the 350 (CAB) PMRL experimental steels [welding parameters: voltage - 35, speed - 9.33/mm/s, submerged arc process ($\eta = 0.95$) ambient temperature - 20°C, uniform preheat - plate dimensions - 500 x 350 x 25 mm, stress concentration $K_t = 3.5$, HIIW hydrogen - 25 ml/100 g, restraint - 400 N/mm³, yield level - 500 mPa].

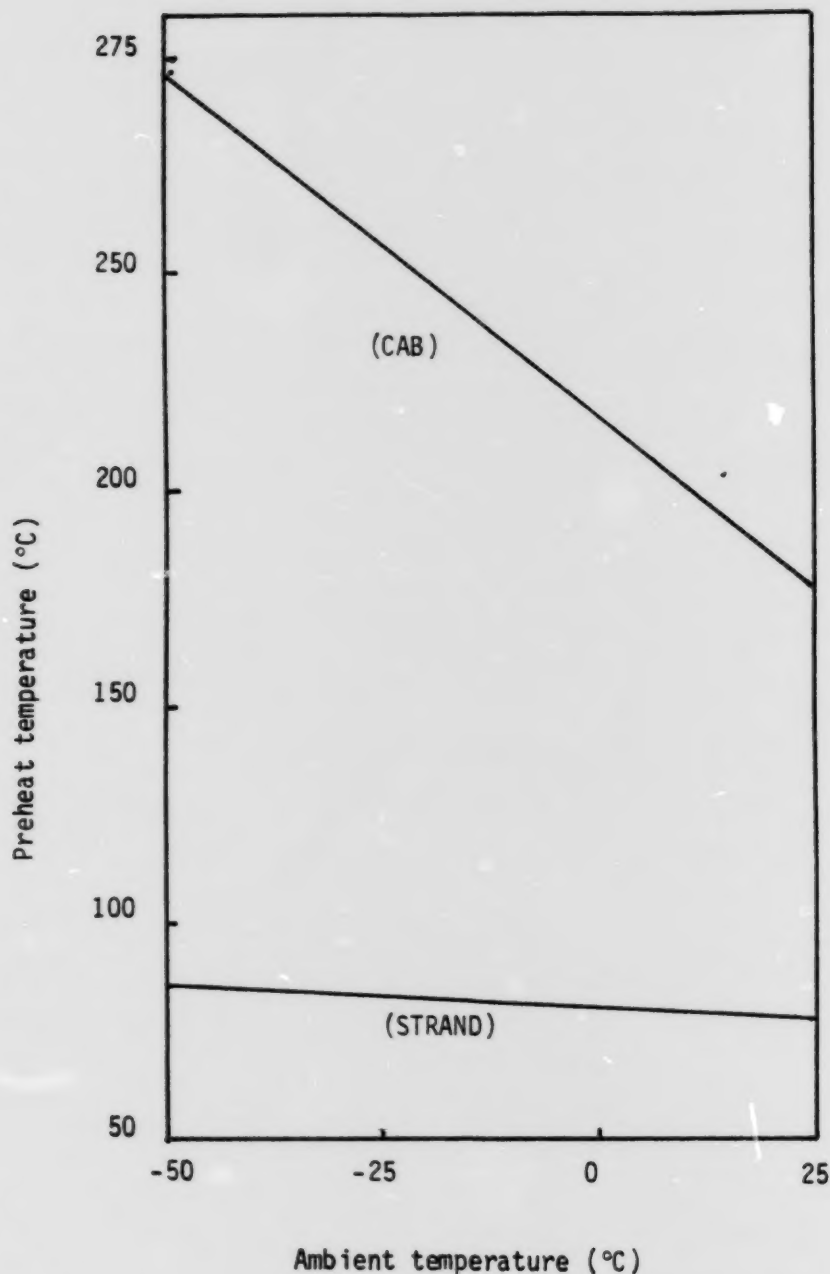


Figure 6 - Effect of ambient temperature on the preheat level for the 350 (STRAND) and the 350 (CAB) PMRL experimental steels [welding parameters: voltage - 35 volts, speed - 9.33 mm/sec, current - 200 amps, submerged arc (η - 0.95) uniform preheat, specimen dimensions - '500 x 350 x 25 mm, restraint - 400 N/mm², yield level - 500 mPa, stress concentration - 3.5, hydrogen level (HIIW) - 25 ml/100 g.]

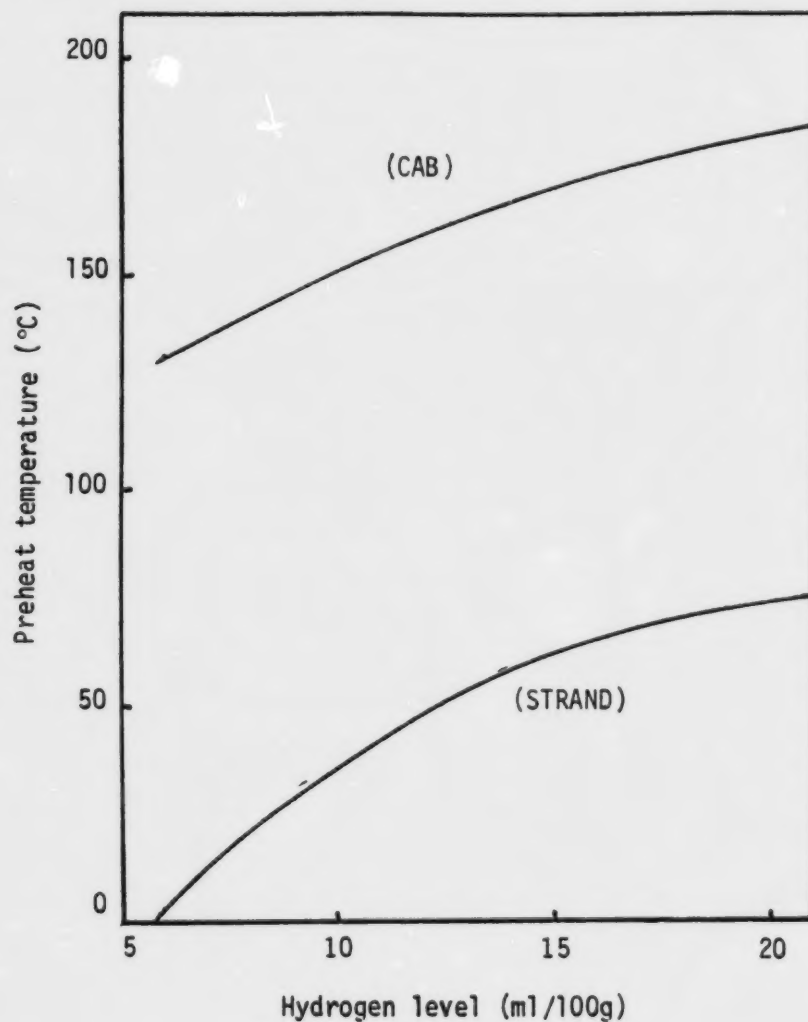


Figure 5 - Effect of hydrogen level (HIIW) on the preheat temperature for the 350 (STRAND) and the 350 (CAB) PMRL experimental steels [welding parameters: voltage - 35 volts, speed - 9.33/mm/s, current - 200 amps submerged arc ($\eta = 0.95$), ambient temperature - 20°C uniform preheat, specimen dimensions - 500 x 350 x 25 mm, restraint level - 400 N/mm², yield level - 500 mPa, stress concentration - 3.5].

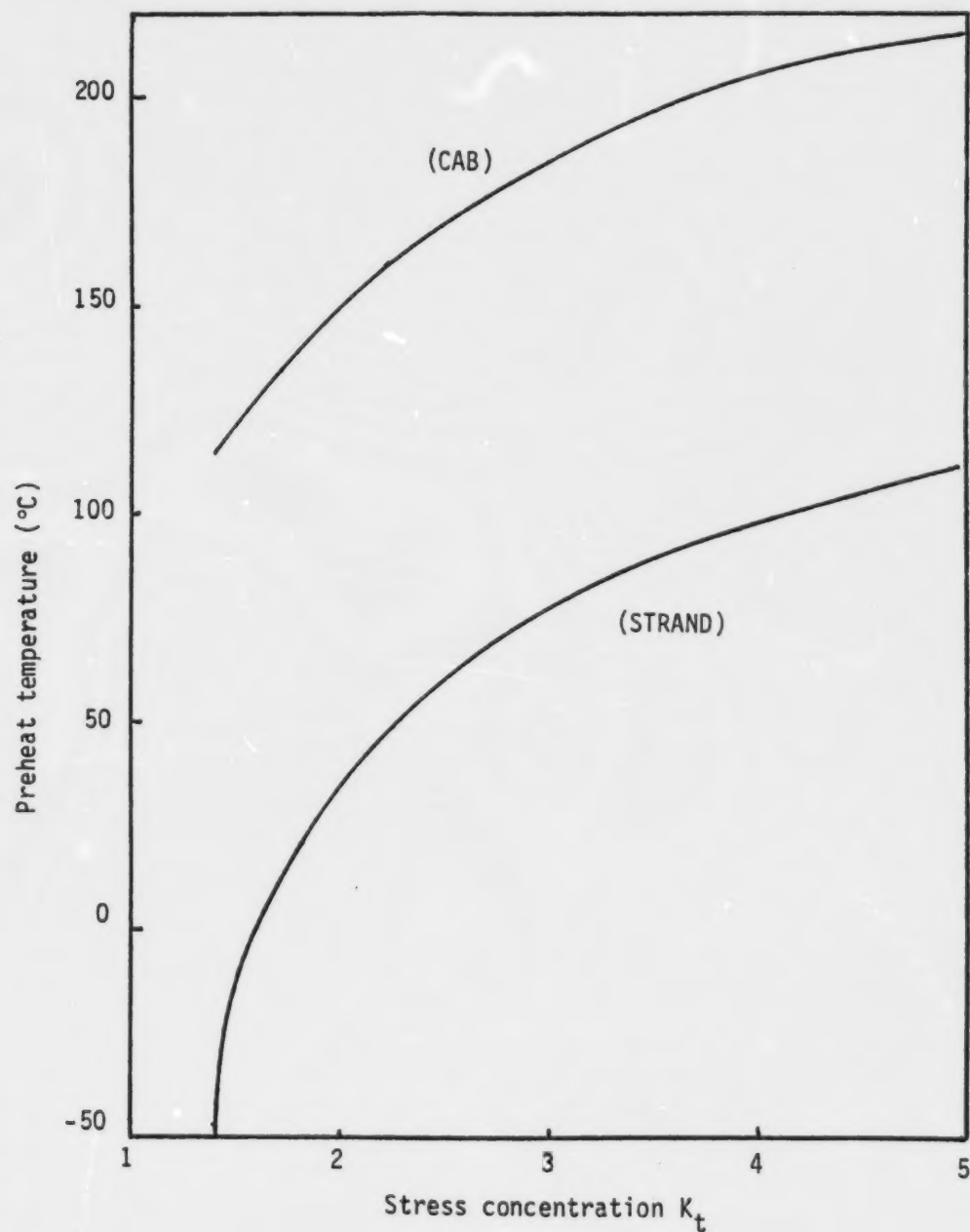


Figure 4 - Effect of stress concentration on the preheat temperature for the 350 (STRAND) and the 350 (CAB) PMRL experimental steels [welding parameters: voltage - 35 volts, welding speed - 9.33/mm/s, current - 200 amps, submerged arc process ($\eta = 0.95$) ambient temperature - 20°C, uniform preheat, plate dimensions - 500 x 350 x 25 mm, hydrogen level (HIIW) - 25 ml/100 g, restraint - 400 N/mm³, yield level - 500 mPa]

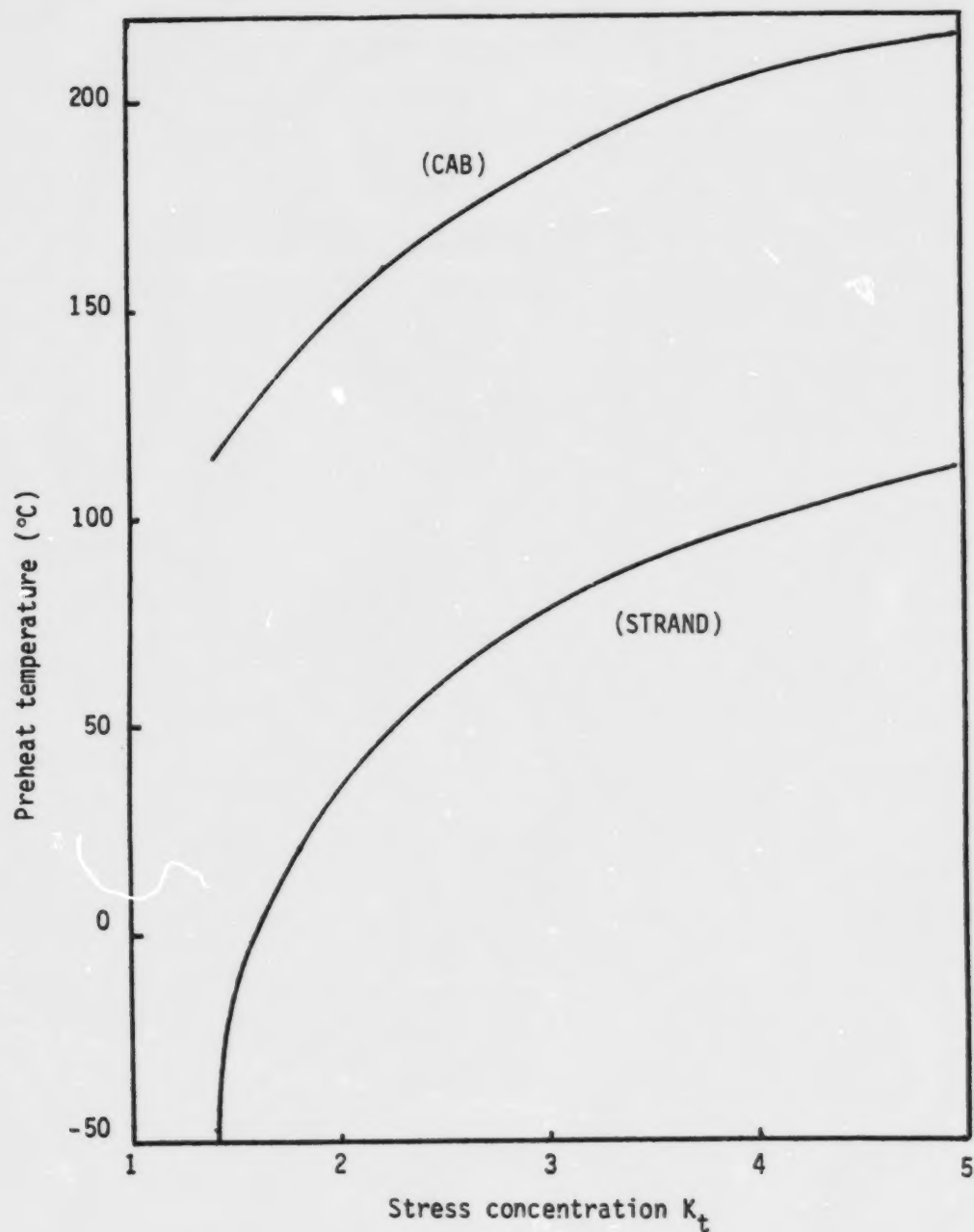


Figure 4 - Effect of stress concentration on the preheat temperature for the 350 (STRAND) and the 350 (CAB) PMRL experimental steels [welding parameters: voltage - 35 volts, welding speed - 9.33/mm/s, current - 200 amps, submerged arc process ($\eta = 0.95$) ambient temperature - 20°C, uniform preheat, plate dimensions - 500 x 350 x 25 mm, hydrogen level (HIIW) - 25 ml/100 g, restraint - 400 N/mm², yield level - 500 mPa]

APPENDIX C

Contained in Appendix C are four papers published during the course of this work, and four presentations on the subject matter of the contract.

Computational Developments In The Watt Transient HAZ Microstructure Algorithm

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10 February 1988

Abstract

Computational developments for implementing the Watt [1,2] HAZ transient microstructure algorithm are presented. Austenite grain size is computed by integrating the grain growth equation along the active region of the thermal path. Similarly, ferrite, pearlite and bainite phase fractions are determined by integrating the Kirkaldy [3] reaction rate differential equations in the appropriate section of the thermal cycle. It is shown that modern high order adaptive ODE solvers provide the best accuracy and efficiency for integrating these equations. Isothermal calculations are presented to demonstrate that computational efficiency can be increased two orders of magnitude by using more effective solver techniques. A discussion of extending this approach to non-isothermal cooling situations is included.

Proceedings of the Modelling of Casting and Welding Processes IV,
Palm Coast, Florida, April 21-27.1988, published as a proceedings
by the Engineering Foundation (U.S.), New York.

Introduction

The heat-affected zone (HAZ) is well known to be the most sensitive area of a weld. The mechanical properties of this region are generally inferior to those of the base metal. In addition the HAZ is generally susceptible to crack formation. The fundamental cause of these problems is the formation of undesirable microstructures (primarily martensite) that result from the thermal cycle.

In recent years three methods have been proposed for computing microstructures in the HAZ. The simplest approach comes from work carried out at the Nippon Steel Laboratories by Yurioka et al [4]. It is a method for calculating the martensite content in the HAZ immediately adjacent to the weld metal. A regression analysis of a large set of HAZ hardness data was used to generate this model. Relationships have been proposed to calculate the maximum cooling time (time for the weld to cool from 800 to 500 C) for 100 % martensite and the minimum cooling time for 0 % martensite. For cooling times beyond the 0 % limit there is no martensite in the structure whereas the structure is all martensite when the weld cooling time is less than the 100 % limit. In between these two limits a logarithmic interpolation is proposed to determine the structure. An algorithm to implement this model is straightforward and there are no special computational difficulties.

A more comprehensive model based on first principle calculations comes from the work of Ion, Easterling, and Ashby [5,6]. They use fundamental kinetics to calculate austenite grain growth and then incorporate the Johnson-Mehl relationships for calculating ferrite, pearlite, bainite and martensite phase fractions. This model is important because it is the first to bring fundamental metallurgical principles to bear on the problem. There are no particular computational difficulties with this model although these authors were graciously given a copy of Ion's original thesis work which is more detailed and clarified some of the material in the original Acta. Met. publications [7].

A third method for computing HAZ microstructures has been proposed by Watt et al [1,2]. They suggest an algorithm that combines Ashby [6] grain growth kinetics with the austenite decomposition reaction rate theory originally proposed by Kirkaldy [3]. Both the grain growth and the phase fraction formulations appear as ordinary differential equations (ODE's) in this method which must be integrated numerically along the time temperature path. The result of this is that microstructures can be tracked throughout the entire thermal cycle. This, in turn, permits the opportunity of coupling microstructure dependent thermal and mechanical properties to FEM temperature and stress computations.

In the following presentation the Watt algorithm is reviewed with particular emphasis on the mathematical ramifications and solution techniques. While implementing the algorithm is relatively straightforward in principle, it can be unreasonably CPU intensive if simple Euler integration is used to evaluate the austenite decomposition equations. Higher order adaptive integration techniques are shown to be considerably more effective.

The Watt Algorithm

The Watt algorithm is best developed for any arbitrary HAZ position with the help of a schematic thermal cycle such as that shown in Figure 1. Equilibrium is assumed during heating and simple lever law computations are applied. In the temperature range $RT < T < A_1$ (heating) the

structure is ferrite(X_f) and pearlite(X_p) given by:

$$X_f = \frac{C_s - C}{C_s} ; X_p = 1 - X_f \quad (1)$$

C_s is the eutectoid carbon concentration(%) which can be taken from the relationship proposed by Leslie [8]:

$$\begin{aligned} C_s &= \frac{[\phi_1 - \phi_2 - A_1]^2}{203^2} \\ \phi_1 &= 910 - 15.2Ni + 44.7Si + 104V + 315Mo + 13.1W \\ \phi_2 &= 30Mn + 11Cr + 20Cu - 700P - 400Al - 120As - 400Ti \end{aligned} \quad (2)$$

The eutectoid isotherm temperature A_1 can be calculated from the relationship [8]:

$$A_1 = 723 - 10.7Mn - 16.9N + 29.0Si + 16.9Cr + 290As + 6.4W \quad (3)$$

In the temperature range $A_1 < T < A_3$ (heating) the structure is ferrite(X_f) and austenite(X_γ) given by:

$$X_f = \frac{C_\gamma - C}{C_\gamma - C_\alpha} ; X_\gamma = 1 - X_f \quad (4)$$

C_α and C_γ are the carbon concentrations(%) in equilibrium ferrite and austenite respectively. They are phase diagram quantities but may be calculated by equation for computer implementation [8]:

$$C_\alpha(T) = 0.105 - 115 \times 10^{-6}T \quad (5)$$

$$C_\gamma(T) = \frac{[\phi_1 - \phi_2 - T]^2}{203^2} \quad (6)$$

The upper critical A_3 can be calculated from the relationship [8]:

$$A_3 = \phi_1 - \phi_2 \quad (7)$$

In the temperature range $A_3 < T < T_s$ (heating) the structure is all austenite. In addition to phase fraction it is also necessary to track austenite grain size. This is because hardenability and

therefore the microstructures formed on cooling are very sensitive to grain size. The as-formed

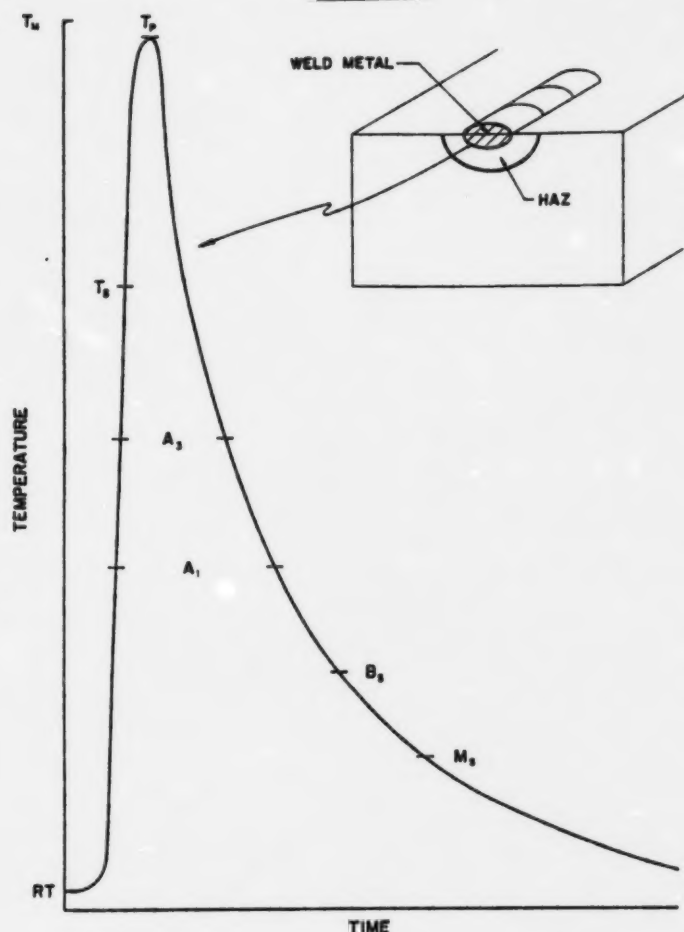


Figure 1: A schematic HAZ thermal cycle to show the regions defined in the Watt algorithm

austenite grain size is assumed to be 5 to 10 microns, which for a modern microalloy steel, does not change in this temperature range. This assumption is appropriate for most modern structural steels that contain grain stabilization alloying, primarily Nb and/or Ti. T_s is the dissolution temperature where the stabilization precipitates dissolve and grain growth begins. T_s is given by a relationship of the form [6]:

$$T_s = \frac{B}{A - \log[C_m^a C_c^b]} \quad (8)$$

The constants A and B depend on the type of precipitate. For NbC they are 3.11 and 7520 respectively [6]. C_m and C_c are concentration (%) metal and carbon (if the precipitate is a carbide) respectively. a and b are the stoichiometric constants for the precipitate in question.

Between T_s (heating) and A_3 (cooling) the structure is austenite but the grain size increases according to the growth equation [6]:

$$\frac{dg}{dt} = \frac{k}{2g} \exp\left(-\frac{Q}{RT}\right) \quad (9)$$

Q is the activation energy (J/mole) for grain growth; k is the growth constant (mm^2/s); t is time; T is absolute temperature, and R is the gas constant ($\frac{\text{J}}{\text{moleK}}$).

In the temperature range $A_3 > T > A_1$ (cooling) austenite begins to decompose to ferrite. The reaction drives toward equilibrium ferrite $[X_{fe}(T)]$. However, ferrite formation is controlled by kinetics according to the relationship [3]:

$$\frac{dX}{dt} = \frac{2^{\frac{(G-1)}{2}} (\Delta T)^3 \exp\left(-\frac{23500}{RT}\right)}{59.6Mn + 1.45Ni + 67.7Cr + 24.4Mo} X^{\frac{2(1-X)}{3}} (1-X)^{\frac{2X}{3}} \quad (10)$$

X is what Kirkaldy [3] calls the phantom fraction ferrite defined as X_f/X_{fe} where X_f is the actual fraction ferrite; G is the ASTM grain size number for austenite; ΔT is the undercooling ($A_3 - T$). The equilibrium ferrite X_{fe} is calculated from the lever law relationship of Equation 1. The result of decomposition in this region is that the structure at any point consists of ferrite (equation 10) and austenite.

In the temperature range $A_1 < T < B_s$ (cooling) pearlite begins to form from austenite which has not yet decomposed to ferrite. Like ferrite the pearlite transformation drives toward equilibrium $[X_{pe} = 1 - X_{fe}]$, but is controlled by kinetics according to the relationship [3]:

$$\frac{dX}{dt} = \frac{2^{\frac{(G-1)}{2}} (\Delta T)^3 D}{1.79 + 5.42(Cr + Mo + 4MoNi)} X^{\frac{2(1-X)}{3}} (1-X)^{\frac{2X}{3}} \quad (11)$$

X is the phantom fraction pearlite X_p/X_{pe} where X_p is the actual pearlite fraction. The eutectoid composition is used to calculate equilibrium pearlite. The ferrite transformation continues in this region but the equilibrium ferrite now becomes $X_{fe} = 1 - X_{pe}$. D is a diffusion parameter evaluated as follows:

$$\frac{1}{D} = \frac{1}{\exp\left(-\frac{27800}{RT}\right)} + \frac{0.01Cr + 0.52Mo}{\exp\left(-\frac{37000}{RT}\right)} \quad (12)$$

In principle ferrite formation stops when pearlite begins to form in accordance with CCT behavior. However, it is difficult to fix the beginning of pearlite formation and therefore, the ferrite reaction is stopped when $X_p = 0.01$. As a result of decomposition in this region the structure becomes ferrite, pearlite and unreacted austenite if the transformation is not complete.

B_s is the bainite start temperature which can be calculated from the following [3]:

$$B_s = 656 - 58C - 35Mn - 75Si - 15Ni - 34Cr - 41Mo \quad (13)$$

In the range $B_s > T > M_s$ (cooling) ferrite and pearlite formation stop and austenite decomposes to a bainite structure according to the kinetic relationship [3]:

$$\begin{aligned} \frac{dX}{dt} &= \frac{2^{\frac{(G-1)}{2}} (\Delta T)^3 \exp\left(-\frac{27800}{RT}\right)}{0.0001(2.34 + 10.1C + 3.8Cr + 19Mo)Z} X^{\frac{2(1-X)}{3}} (1-X)^{\frac{2X}{3}} \\ Z &= \exp[X^2(1.9C + 2.5Mn + 9Ni + 1.7Cr + 4Mo - 2.6)] \end{aligned} \quad (14)$$

X is the bainite fraction formed and ΔT is undercooling. It should be noted that Z is set to 1 for all negative values of the exponent. Initially the bainite fraction is set to a ghost level equal to the pearlite fraction as suggested by Kirkaldy[3]. Apparently pearlite provides active

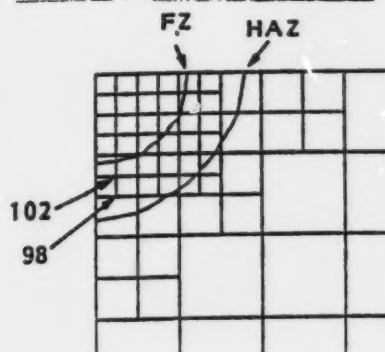
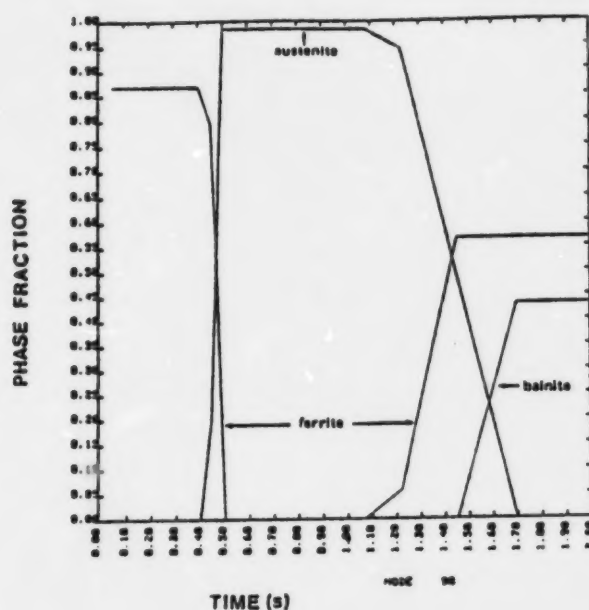


Figure 2 Transient microstructure changes in the HAZ of a small bead-on-plate weld; heat input - 0.21KJ/mm, base metal composition: 0.12C, 0.91Mn, 0.16Si, 0.04Al, 0.021Nb, 0.011N, 0.002P, 0.005S (Note - experimental work on this weld can be found in the PhD thesis of Ion, Lulea, Sweden, 1984, reference 7).

nucleation sites for bainite and therefore stimulates initial formation. In the event that some of the austenite has not yet decomposed the structure in this region consists of ferrite, pearlite, bainite and unreacted austenite.

The M_s temperature may be calculated from the relationship [3]:

$$M_s = 561 - 474C - 35Mn - 17Ni - 17Cr - 21Mo \quad (15)$$

When the M_s temperature is reached all remaining austenite is assumed to transform to martensite. This is a reasonable assumption for most structural steels but should be modified to account for retained austenite for richer machine and tool steels.

To calculate the HAZ structure for a given situation the Watt algorithm is coupled to a cooling model, usually FEM based. The transient microstructure for a HAZ position adjacent to a small weld on an off-shore steel plate is shown in Figure 2.

Integration Considerations

Integrating the reaction rate equations along the thermal path can be prohibitively CPU intensive. Reaction rate equations are highly non-linear (see Figure 3) and simple Euler integration is inefficient in such situations. Small time increments are necessary when growth is rapid to ensure accuracy but is not necessary in the beginning (nucleation) or when growth is nearly complete. At the same time it is not possible to anticipate where growth will be rapid. This suggests that adaptive solution techniques where increment size is automatically adjusted to preserve numerical accuracy should be used.

To demonstrate the problem consider the solution to Equation 10 for simple austenite to ferrite decomposition at 650 C. The steel in this case has a grain size of ASTM 8.54 and a composition: 0.12C, 0.91Mn, 0.16Si, 0.021Nb, 0.04Al, 0.002P, and 0.005S. The A_3 temperature for this

Table I

Effect of Time Step Size on the Number of Evaluations Necessary to Solve the Isothermal Decomposition Problem

Time Step (seconds)	Ferrite Fraction Formed: $X(0.5)$	Number of Evaluations
0.1	0.0033	5
0.01	0.2649	50
0.001	0.4018	500
0.0001	0.4215	5000
0.00001	0.4213	50000

Notes

- (1) Isothermal decomposition temperature - 650 C
Austenite ASTM grain size - 8.54
Equilibrium ferrite fraction - 0.86
Steel composition: 0.12C, 0.91Mn, 0.16Si, 0.021Nb, 0.04Al, 0.002P, 0.005S, 0.011N
 A_3 critical temperature - 836 C
- (2) Initial fraction ferrite - $\epsilon = 10^{-13}$

material is 836 C and the equilibrium ferrite is $X_{f_e} = 0.86$. This situation is presented because it arises as a result of study on the transient microstructure computations shown in Figure 2. Formulating the problem from a real welding situation ensures that the results are relevant to HAZ decomposition.

The austenite to ferrite decomposition for this particular situation is shown in Figure 3. To compare solvers the fraction ferrite formed in 0.5s ($X = 0.42$ to two significant figures) is selected for study. If the simple Euler method is used to compute the ferrite fraction, an initial value $X(0)$ must be assigned. It is not possible to start integrating at $X(0) = 0$ because this produces the trivial solution $X(t) = 0$. The obvious alternative is to set $X(0) = \epsilon$ where ϵ is a sufficiently small number. In addition the time step must be small enough to ensure convergence. Surprisingly two digit accuracy was not achieved with the simple Euler solver until $\epsilon < 10^{-10}$ and $\Delta t < 10^{-4}$ as shown in Tables I and II. In this particular situation at least 5000 evaluations are necessary to achieve two digit accuracy. It is apparent that CPU time can rise rapidly for HAZ computations where several transformations must be tracked at several hundred points in the region.

Starting Condition

While the initial fraction ferrite $X(0)$ assumed does not affect the number of evaluations directly it must be small enough to ensure sufficient accuracy (two digit in this case). Alternatively, Equation 10 can be replaced with an asymptotic approximation until $X(t)$ is sufficiently large and then switched to the full form solution to complete the calculation. Equation 10 can be written in the general form as follows:

Table II

Effect of Initial Increment Size on the Accuracy of the Solution to the Isothermal Problem

Initial Fraction Ferrite: $X(0)$	Fraction Ferrite Formed: $X(0.5)$
10^{-2}	0.7916
10^{-4}	0.5027
10^{-6}	0.4406
10^{-8}	0.4260
10^{-10}	0.4217
10^{-12}	0.4213

Notes

- (1) Isothermal decomposition parameters described in Table I notes.
- (2) Time step selected for evaluation - 0.0001 s

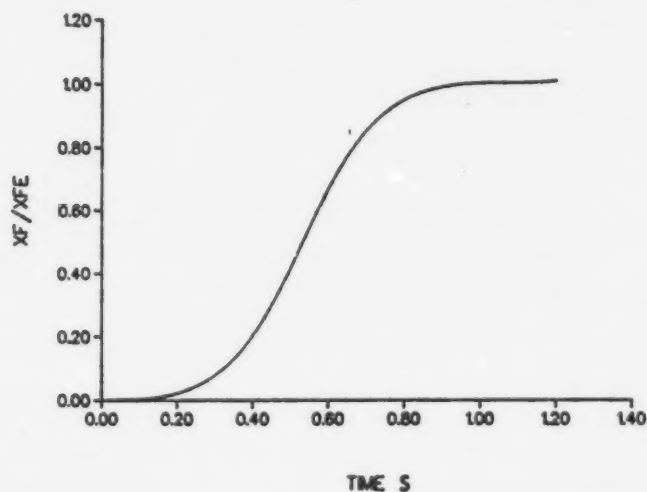


Figure 3 Isothermal ferrite formation from austenite at 650 C for a steel with base composition: (see Figure 2 caption); an austenite grain size of ASTM 8.54, $A_3 = 836$ C, $A_1 = 718$ C, and an equilibrium ferrite fraction $X_{fe} = 0.87$.

$$\frac{dX}{dt} = AX^{\frac{1}{2}}(1-X)^{\frac{1}{2}} \quad (16)$$

An asymptotic approximation to Equation 10 can be written as:

$$\frac{dX}{dt} = AX^{\frac{1}{2}} \quad (17)$$

This satisfies the initial condition $X_f(0) = 0$; yet Equation 17 has an analytical solution:

$$X(t) = \left(\frac{At + K}{3} \right)^3 \quad (18)$$

where K is the integration constant which is 0 when the boundary condition $X(0) = 0$ is applied and becomes:

$$X(t) = \frac{At^3}{27} \quad (19)$$

In practice Equations 10 and 19 are used together to obtain the phase fraction ferrite formed. The integration begins with Equation 19 and is then switched to Equation 10 when $X(t)$ is sufficiently large. In this particular case the switch is made at 0.01s.

The Time Step Problem

The efficiency of the numerical integration can be increased considerably by using contemporary methods that include adaptive time stepping and automatic error checking. The adaptive Euler, the second and fifth order Runge-Kutta methods, and the Adams-Bashforth adaptive solver were selected for study. They are well known, well documented [9,10] and since they can be obtained from the Slatec library of mathematical routines [11] coding is not an issue. All codes control the local error by specifying a tolerance typically 10^{-6} . The code advances the solution from the starting condition t_{in} in Equation 10 to t_{out} using step sizes which are automatically selected to keep the local error in each step within tolerance.

The results of using higher order methods to evaluate the isothermal decomposition problem are shown in Table III. The advantages are obvious. The computational efficiency is increased by almost two orders of magnitude with the Adams adaptive method. However, a tolerance of 10^{-6} seems necessary to achieve two digit accuracy for most of the austenite decomposition problems tested by these authors. While the advantages of using higher order solvers to evaluate austenite decomposition have been demonstrated for isothermal decomposition the situation is not as straightforward for HAZ microstructural computations where non-isothermal cooling is involved. In this case the temperature (T) and the equilibrium fraction ferrite (X_{fe}) change with time in Equation 10. In principle, even the grain size G can increase during decomposition although this is insignificant in practice. The algorithm has not yet been fully implemented to accept higher order solvers for HAZ microstructural computations. Work is progressing in this area.

Conclusions and Contributions

- (1) The Watt algorithm for computing transient HAZ microstructures has been reviewed.

Table III

Comparison of ODE Solvers For Integrating The Isothermal Decomposition Problem

	Euler Non-Adaptive	Euler Adaptive	Runge-Kutta Second Order	Runge-Kutta Fifth Order	Adams Adaptive
$X(0.5)$	0.4217	0.4102	0.4157	0.4160	0.4160
Number of Evaluations	5000	702	685	298	71

Notes

- (1) Values are fractions ferrite at time=0.5s - see Figure 3
- (2) See Table I notes for problem definition
- (3) Tolerance= 10^{-6}

(2) The computational advantages of using higher order adaptive solvers for integrating the reaction rate equations have been demonstrated.

Acknowledgements

The support of the National Science and Engineering Research Council: NSERC A4901 (M. Bibby) and NSERC A2922 (J. Goldak) are gratefully acknowledged.

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A methodology for computing heat affected zone hardness, microstructure and preheat temperature

M.J. Bibby, J.A. Goldak and I. Jefferson (Carleton University) and
J. Bowker (Energy, Mines & Resources — Government of Canada)

SUMMARY

The principles used to compute as-welded HAZ hardness, post weld heat-treated HAZ hardness, HAZ microstructure fractions and preheat temperatures to avoid underbead cold cracking are reviewed. Comparative calculations are presented for seven as-welded HAZ hardness models, six microstructure/hardness models and two HAZ reheat hardness models. These, in turn, are compared to measured values. In addition, an algorithm based on the Nippon Steel model for computing preheat temperature to avoid HAZ underbead cold cracking is included. The results of this study suggest that because of uncertainties in the calculations a computer system consisting of several models should be used as a basis for engineering judgement in practice. While this presentation deals primarily with HAZ computational software, progress in research to provide a user friendly welding engineering computer environment is reported.

INTRODUCTION

In recent years weld process modelling to predict the properties of the heat-affected zone (HAZ) has received considerable attention. Steel producers are interested in such models because they provide a theoretical framework for predicting how a new steel chemistry will respond to the welding process. Welding engineers and fabricators can make use of these developments when design specifications must be met. For example, it is relatively common practice to impose a hardness limit of 280 VPN on the HAZ in situations where stress corrosion cracking is anticipated (nuclear reactors, sour gas linepipe applications, etc.) [1]. Models available for computing HAZ hardness and post weld heat treated (PWHT) hardness can be used as a guide for selecting steel compositions and welding parameters to meet this specification.

In addition to weld hardness, models have been proposed recently for computing HAZ microstructures. The volume fraction of martensite is the most significant component since this is the microstructural component that poses the most danger in practice. Microstructure computations are fundamental to predicting the behaviour of the HAZ and may be viewed as a basis for all other computations (strength, toughness, hardness, cold crack formation, etc.). Even in the absence of property calculations, an experienced metallurgist can use the microstructure computations as a basis for evaluating the risk of catastrophic problems in service.

Over and above hardness and microstructure, a model that includes the effect of hydrogen has been developed at Nippon Steel Laboratories for predicting the appearance of cold cracks. By combining this algorithm with a suitable weld cooling model preheat levels to avoid cold crack formation can be computed.

While there is little doubt about the potential value of weld models, they are often not routinely used because the computations are lengthy. Computer implementation is the obvious answer to this limitation but this must be approached with some care. If computer software is to win a place in routine design and fabrication practice, it must be developed for a welding engineering environment. In particular the software should be arranged with a convenient user interface, preferably good output graphics and a reasonable input database. It is important that these should be developed by engineers active either in welding research or practice to take advantage of experience and customs unique to the profession.

COMPUTING HAZ HARDNESS

Hardness has always been an important property for assessing weldability [1]. This is largely because it is easily measured and is local enough to probe the small sensitive area of the HAZ immediately adjacent to the weld metal. Some fourteen models have been proposed in the literature for computing as-welded HAZ hardness [2-18]. They may be classified into two relatively independent groups designated in this presentation as the regression models and the microstructure models. The regression models, as the name implies, are the result of statistical analyses of measured results. In the microstructure models hardness is a secondary calculation. Microstructure fractions are first calculated and then a law of mixtures is applied to generate HAZ hardness.

While all of the regression models are the result of independent statistical analyses, they are nevertheless, all based on the same physical principles. A "characteristic hardening curve" (CHC) is assumed to exist that describes the HAZ hardening response of a material to the welding process [3]. The CHC is unique for a given chemistry and may be viewed as a property of the material. A CHC hardening curve for a low carbon off-shore steel is shown in Fig. 1. It is a plot of HAZ hardness against cooling time (800 to 500 °C). CHC curves are typically determined from the measurements of a series of bead-on-plate welds. The cooling time is usually measured by injecting a high temperature thermocouple into the molten pool. The HAZ hardness is measured by taking a series of independent measurements at different locations in the HAZ along the length of the weld.

There is some doubt that a unique hardness exists for the HAZ of a given weld. Considerable variation might be expected along the length because of heat source instabilities or around the cross-sectional periphery due to variations in cooling rate. In fact, there is little variation in hardness along the length or around the cross-sectional periphery of a weld deposited with a reasonably well controlled process (Figs. 2 and 3). There is less than 10 VPN variation along the length of the autogenous electron beam welds shown in Fig. 3. An autogenous weld was selected to demonstrate consistency because the hardness of the weld metal is the same as that of the HAZ (Fig. 2). Similar consistency is found around the cross-sectional periphery of such a weld.

The scatter found with most HAZ hardnesses reported is not inherent but rather there is difficulty with the measurement. It is a spatial resolution problem. Positioning the indenter precisely in the small region of maximum hardness is a problem and even then there often is insufficient high strength material surrounding the indentation to support the diamond properly. This is particularly true of small welds where the hardness is high. In this case it is often preferable to use autogenous electron beam welds. The electron beam process is preferred because the heat source efficiency is well known (0.9) and is consistent. In an autogenous weld the weld metal has the same hardness as the coarse grained HAZ region in most cases. Therefore there is high strength material supporting the indentation at least on the weld metal side.

Then too, there is reason in principle to believe that HAZ hardness is reasonably consistent. The CHC is best represented as a logarithmic time plot (see Fig. 1). Therefore a relatively large fluctuation in

cooling time($\pm 20\%$) causes only a small change in HAZ hardness.

The first reference to a CHC seems to be Stout's early work at Lehigh in 1946 [2]. In recent years Japanese researchers have made frequent reference to the concept and use it as a basis for HAZ hardness models. The technique involves suggesting a mathematical form that describes the shape of the CHC. Beyond this CHC curves for several chemistries are measured and multiple regression techniques are used to fix the coefficients of the general mathematical relationship that generates the curve for any particular material composition.

WELD COOLING MODELS

To predict the HAZ hardness in any given welding situation it is also necessary to compute the cooling time from the welding parameters. The cooling time is then applied to the CHC (see Fig. 1) to determine the HAZ hardness. There are two extremes for computing the cooling time - the simplistic Adams relationships on the one hand and comprehensive FEM computations on the other. The Adams point source model contains several assumptions that limit the sensitivity and accuracy of the computations[19]. Modifications to the Adams/Rosenthal theory have been proposed to eliminate some of the more important approximations[15]. However, it is these authors' experience that such intermediate models do not offer significant improvement beyond the Adams approach. On the other hand, FEM analysis is quite another matter since joint and workpiece geometry, thermal properties that vary with temperature, the heats of fusion and transformation, surface losses, and a volume heat source can all be incorporated in the computation[20]. Comparative calculations for a 3kJ/mm bead-on-plate weld are contained in Table 1. The specifics of the calculations (mathematical relationships and limits) are contained in references 19-21.

Included also in Table 1 is the cooling time calculated with the Kohira cooling model which is intermediate. Basically it is the point source Adams/Rosenthal approach but contains a surface heat transfer (loss) coefficient. As shown in Table 1 this seems to make little difference (Adams-18s, Kohira-18.3). This is generally the case where cooling times are less than 20s. However, for welding situations where the cooling time exceeds 20s, surface heat losses become significant. These authors would suggest this as a limit for Adams cooling time computations.

The cooling time computations shown in Table 1 would suggest that there is not a great deal of difference between the Adams and FEM approaches. However, an artificially low value for thermal conductivity of 22 W/m °C (see Fig. 4) was used in the Adams method to ensure this agreement. In fact the thermal conductivity parameter in this case has no physical meaning and is used simply as a mathematical coefficient (with units of W/m °C) to match measured and calculated values. It has been shown that to some extent a low thermal conductivity parameter compensates for several model assumptions in the Adams approach[21]. This is, of course, dangerous practice because such a match is not always assured. Nevertheless, many welding engineers and researchers have used and will continue to use the Adams approach because of its simplicity. In so doing a thermal conductivity value of 22 W/m °C is recommended based on these authors' experience and the experience of others.

A COMPARISON OF HAZ HARDNESS COMPUTATION METHODS

Computed HAZ hardness values for a low carbon off-shore steel weld using seven of the regression models available for this purpose are shown in Table 1. The details (mathematical relationships and limits) are contained in references 3-11. There is remarkable consistency for the Arata, Dueren, Suzuki, Teresaki and Yurioka models I and II. The Cottrell and Beckert models are high and low respectively

Table 1: Cooling Time and Hardness Computations for a 3KJ/mm Submerged Arc Weld

Cooling Time Model (1, 2)	Adams 18s	Kohira 18.3s	FEM (6) 16.6s to 19.6s	
Hardness Model (3, 4, 5)				
Arata	248.2	247.6	251.2	245.1
Beckert	216.3	215.8	219.2	213.8
Cottrell	287.3	286.1	293.1	281.0
Dueren	248.1	246.9	254.2	241.7
Suzuki	249.5	248.7	253.8	245.3
Terasaki	248.1	247.7	254.0	243.6
Yurioka I	254.1	253.1	259.3	249.1
Yurioka II	242.9	242.4	245.8	240.0

Notes

- (1) Measured cooling time: 20 s
- (2) See references 19-21 for cooling time model details
- (3) Measured HAZ hardness: 252 VPN
- (4) See references 3-11 for hardness model details
- (5) Base metal composition: 0.12C, 1.29Mn, 0.28Si 0.15Cr, 0.14Ni, 0.10Mo, 0.05V, 0.16Cu, 0.03Nb, 0.008S, 0.007N, 0.015P
- (6) Hardness computed at the extremes (16.6s and 19.6s).

for this particular situation. The consistency of the five models strongly suggests a probable HAZ hardness of about 250 VPN. In fact the measured hardness is 252 VPN. Model consistency seems to be relatively general for several off-shore compositions ($0.05 < C < 0.15$) examined by these authors at this heat input level (3kJ/mm).

However, this kind of computational ordering does not always occur. What is recommended by these authors is a computer system that incorporates several models such as the seven methods used to generate the data in Table 1. By computing several HAZ hardnesses for each situation engineering judgement can be applied to estimate a reliable value. On the other hand it is dangerous to rely on any one model.

THE MICROSTRUCTURE HAZ HARDNESS MODELS

In these models the calculation strategy is to generate an algorithm for computing the HAZ microstructure mix and then apply a law of mixtures to compute the hardness. There are essentially three approaches arising from the work at Creusot-Loire[12,13], the work at Lulea, Sweden [14,15] and the Canadian work at the Universities of Windsor and Carleton[16,17]. In addition to this the volume fraction of martensite can be computed from the Arata[3] and Yurioka[7,18] regression model. The mathematical relationships and specifics of all of these models are contained in reference 3,7 and 12-18. What follows is a brief discussion of the relevant features of each model and some comparative computations.

The Creusot-Loire system was the first microstructure method. It is based on hardenability prin

ciples. Mathematical relationships have been established for computing the critical cooling rates at 700 °C (equivalent to 300/(cooling time)) for 100% martensite, for bainite-ferrite separation and for 0% martensite. A kinetic time-temperature equivalence parameter is used to take into account the dependence of hardenability on austenite grain size.

The Creusot-Loire system is comprehensive, based on several tens of man-years of experimental CCT work and statistical analysis. However, it applies primarily to steels heat-treated by conventional means where the thermal cycle is well known. It is somewhat more difficult to adapt the method to the continuous thermal cycle of a HAZ. In fact austenitizing conditions of 1s at 1400 C are assumed for the coarse grained HAZ position next to the deposit of all welds. While this may seem dangerous, reasonable estimates of microstructure and HAZ hardness are possible (see Table 2).

The austenitizing kinetics of continuous heating and cooling is incorporated in the Ashby, Easterling, Ion method. In addition Johnson-Mehl transformation relationships are applied to compute HAZ microstructures. This represents a considerable advance in applying fundamental principles to the problem. On the other hand, this model is a comparative method that depends on measured HAZ microstructure fractions for each steel chemistry. Once benchmark microstructure fractions are known for one weld heat input they can be computed for any other welding situation.

The Ashby, Easterling, Ion method is a very important development because it is the first microstructure method to apply first principle kinetics to the problem. However, the extent to which this method can be applied in practice depends on the availability of measured values. In addition, only residual HAZ microstructures are computed. In FEM thermal and thermal stress modelling it is necessary to compute transient microstructural changes. Thermal and mechanical properties are associated with each microstructure and this information is then folded back into the computations.

A transient microstructure model has been proposed by Watt et al [16] that does not depend on measured benchmarks. It is based on the fundamental austenite transformation kinetics originally proposed by Kirkaldy [22] which has long been used for hardenability computations in the heat-treating industry. For example, CCT diagrams and Jominy-end-quench hardness curves can be generated from the Kirkaldy system. The austenite decomposition relationships in this scheme are formulated as ordinary differential equations which must be integrated numerically to compute the fraction of each microstructural component formed. This can be CPU intensive if a simple Euler integration scheme is used. An adaptive integration scheme has been suggested to increase computational efficiency [17]. A computed microstructure distribution across a small bead-on-plate weld is shown in Fig. 5 to demonstrate the sensitivity of the system. Similar computations that are transient are possible because the microstructure is tracked around the entire thermal cycle.

The martensite fraction in the coarse grained area of the HAZ region next to the weld metal can also be computed from relationships established in the regression models of Arata, and Yurioka. Essentially critical cooling times for 0% and 100% martensite as a function of composition are computed. If the cooling time in a given welding situation is less than the critical for 100% martensite, the structure is assumed to be fully martensitic. A logarithmic cooling time interpolation is used to compute the fraction martensite between the 0% and 100% critical limits.

Computed HAZ microstructure and hardness values for two gas metal arc welds are shown in Table 2. Computational details are given in references 3,7 and 12-18. It is apparent that there are considerable differences in the computed microstructure values. In addition, it is not obvious which model should be used in practice. In principle the Watt and Ashby models are the most fundamentally based and in the long term this is the best answer. However, uncertainties in the input data limits the significance of the computed values and the reliability at this time is not necessarily greater than that of the regression models. It would appear from the Table that the Yurioka I and Creusot-Loire values agree with the measurements more closely than the values generated with the more fundamental Watt or

Table 2: HAZ Microstructure and Hardness Computations For Two Gas Metal Arc Welds

Computation Method(1)	Cooling Time(s)		Hardness VPN(2)		Fraction Martensite	
	Weld 1	Weld 2	Weld 1	Weld 2	Weld 1	Weld 2
Measured(3)	0.8	2.1	371	347	0.86	0.63
Watt			376	346	1.0	0.80
Ion			343	305	0.76(4)	0.50(5)
Maynier			384	337	1.0	0.64
Yurioka I			376	330	0.83	0.62
Yurioka II			345	272	0.66	0.48
Arata			371	317	0.97	0.78

Notes

(1) Computational methods outlined in references 3,7 and 12-13.

(2) Base metal composition: 0.12C, 0.91Mn, 0.16Si, 0.002P, 0.005S, 0.021Nb, 0.011N, 0.04Al.

(3) Experimental measurements obtained from the thesis work of Ion[23].

(4) Measured benchmark—weld 2.

(5) Measured benchmark—weld 1.

Ion models. However, this is not always the case. Then too, there are experimental difficulties and there is uncertainty in the measured values. It is these authors' recommendation that all model values should be generated by computer and the range used as a basis for estimating the martensite content in any given welding situation.

POST WELD HAZ HARDNESS COMPUTATIONS

There are essentially two models available for computing the HAZ hardness of welds that have been heat-treated after deposition. A tempering model is integrated into the Cruesot-Loire system which can be applied to welding situations[13]. Essentially tempering kinetics are applied to the HAZ microstructure fractions that have been calculated from the primary algorithm. Similarly from the Nippon Steel Laboratories, Yurioka has proposed a tempering model that can be applied to the HAZ[24]. Both softening and hardening (aging) mechanisms are contained in the relationships. Time and temperature are combined (kinetics principles) into a single parameter to account for the effect of both factors on reheat hardness.

Computed as-welded and reheat hardnesses (620 C - 2 hrs.) for two submerged arc welds are reported in Table 3. Computational details are contained in references 12—13 and 24. It is evident that there are considerable differences between the values calculated with these two PWHT models. It is equally obvious that in spite of this the computations are both interesting and potentially very useful. These authors recommend that both computations should be made for any given welding situation and the results used as a basis for applying engineering judgement. Since these are regression models it is not possible to account for all the differences between the calculated values. On the other hand the older Maynier model does not take into account Nb precipitation hardening which can be quite significant. If Nb is extracted from the Yurioka model then the reheat computations are in much better agreement and these, in turn, agree reasonably well with measured values. However, in principle, Nb precipitation

Table 3: HAZ Hardness Computations After Post-Weld Heat Treatment

Model(1)	Cooling Time(2) (s)		Hardness As Welded (VPN)(3)		Hardness PWHT (VPN)(4)	
	Weld 1	Weld 2	Weld 1	Weld 2	Weld 1	Weld 2
Measured	3.1	10	425	310	235	220
Maynier			409	366	232	214
Yurioka			402	321	284	276
					(247 Nb-free 239)	

Notes

- (1) See references 12-13 and 24 for computational details
- (2) Submerged arc welds: cooling times measured by injecting thermocouples into the weld pool.
- (3) Base metal composition: 0.16C, 1.42Mn, 0.3Si, 0.02Ni, 0.03Cr, 0.07Cu, 0.012P, 0.001S, 0.02Nb, 0.006N, 0.03Al.
- (4) Post weld heat-treatment: 620 °C, 2Hrs.

should be included, which once again reinforces the argument that an engineer in practice should not rely on any one computation.

HYDROGEN BASED PREHEAT COMPUTATIONS

HAZ cold cracking, sometimes called underbead cracking, is a well known phenomenon in welding technology. Cracks are caused essentially by residual tensile stresses that form as a result of thermal shrinkage when a weld cools. The residual stress level often exceeds the yield strength of the material which in turn causes plastic flow. When the plastic capacity of the joint region is exhausted cracks can form. The situation is complicated by the simultaneous formation of hardened microstructures of limited plastic capacity. Moreover, it is further complicated by the presence of hydrogen. Hydrogen forms in the arc and is "pumped" into the HAZ through the weld metal. In this model the effect of hydrogen is assumed to dominate the mechanism.

Hydrogen diffuses into the HAZ at high temperatures but escapes as the weld cools. The hypothesis is that a critical level of hydrogen exists in the HAZ below which cold cracks do not form. This critical level depends on composition, joint shape, workpiece size and shape, yield level of the base material and ambient temperature.

In practice preheat is used to slow down the cooling and provide an opportunity for the HAZ hydrogen to drop below the critical level[25]. Hydrogen escapes down to a temperature of about 100 °C. Below this temperature diffusion is so slow that any hydrogen left can be considered to be trapped. At the same time cracks form at temperatures below 100 °C. and therefore the hydrogen environment is fixed before cracking occurs. A critical time is defined in the Yurioka model which is the cooling time to 100 °C. ie the time for hydrogen to drop to the critical level. If the real cooling time is greater than the critical cooling time then cracking is avoided. The real cooling time of the weld is calculated with the help of a long time low temperature heat flow model. Such computations were used to generate the data presented in Fig. 6. This Figure is submitted to show just how useful the system can be

in practice. The preheat level needed to avoid underbead cracking for (a) uniform preheat (b) local preheat with electrical strip heaters is shown. Details of the method are contained in reference 25.

Neither these authors nor, we suspect, Yurioka et al wish to leave the impression that preheat computations are precise—far from it. The cracking mechanism is very complex and it will be some time before it is well enough understood to model it precisely. Nevertheless this model is an important development and the computations form a useful basis for engineering judgement in practice.

There is an alternative to the Nippon Steel method. These authors understand that the Bailey nomogram model [26] has been computerized by the Welding Institute. This, too, is almost certainly a valuable addition to HAZ computational software. As a minimum it provides a second preheat evaluation which is a better basis for judgement in practice than just the Yurioka method. Over and above this the accumulated experience of the Welding Institute cannot be overestimated and much of this is contained in the Coe/Bailey strategy for preventing HAZ cracking. However, at this point in time these authors have not had an opportunity to examine the software or to computerize our own version of the Coe/Bailey method from scratch. It is, therefore, not contained in this presentation.

RANGE OF APPLICABILITY OF HAZ MODELS

Since most of the models (as-welded HAZ and reheat hardnesses, microstructure, and preheat level) are semi-empirical, it is important to know the range of applicability. However, space does not allow exhaustive documentation and discussion. The original papers referenced at the end of this text have to be consulted for details. Nevertheless, in general these models can be applied to plain carbon, microalloy and low alloy steels. The Yurioka II HAZ hardness model is intended primarily for high yield steels ($Ni < 10 \text{ w/o}$, $Cr < 10 \text{ w/o}$).

COMPUTER CONSIDERATIONS

With the exception of FEM all computations can be implemented on a small personal or portable computer. Portable and pocket computers are intentionally included in this list since they can be convenient in a shop environment[27,28]. At present (1987) a relatively powerful workstation (e.g. Sun or Appolo) is required for FEM cooling. It has been said that computing capacity increases one hundred fold every seven years. It will, therefore, not be long before all weld analyses including FEM thermal and thermal-stress computations can be carried out on relatively inexpensive personal workstations.

Up to this point these authors have suggested that because of the semi-empirical, inexact nature of HAZ calculations several models should be incorporated in a computational system. While this is necessary it is not sufficient. If the system is to be used in practice it must be "user friendly". In addition, to weld models the system should have a well designed user interface, a relatively straightforward graphics display and a well organised database. The interface might consist of a series of windows such as that shown in Fig. 7. Each input should be independent of any other input and recomputations should be possible after any change in the data. In addition, relatively flexible graphics should be incorporated in the system and displayed to this same interface. Then, for example, the preheat temperature vs welding current shown in Fig. 6 can be displayed directly in a convenient user friendly form.

In addition to the user interface and graphics, a well organized database can increase the convenience and usability of the system considerably. As a minimum it should contain those steels that are frequently used and must be extendable by the user. It should be arranged so that steel compositions and

other relevant data can be automatically loaded for processing. Frequently the nominal composition is not the actual composition but is useful as a starting point. If the nominal compositions are stored as limits then HAZ hardness and preheat maximums can be computed which will be conservative but useful. If heat chemistries are known then more accurate computations are possible.

CONCLUSIONS

A comparative study of several models available for calculating as-welded HAZ and reheated HAZ hardnesses, microstructures, and preheat levels leads to no general conclusion regarding accuracy. Instead these authors recommend that several models should be incorporated in a computer system and these used as a basis for engineering judgement in practice.

ACKNOWLEDGEMENTS

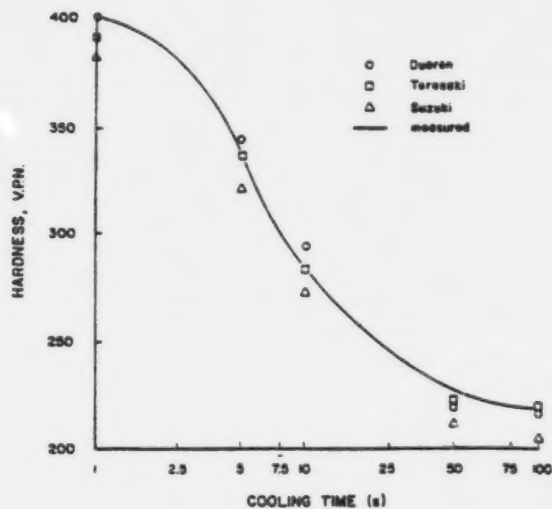
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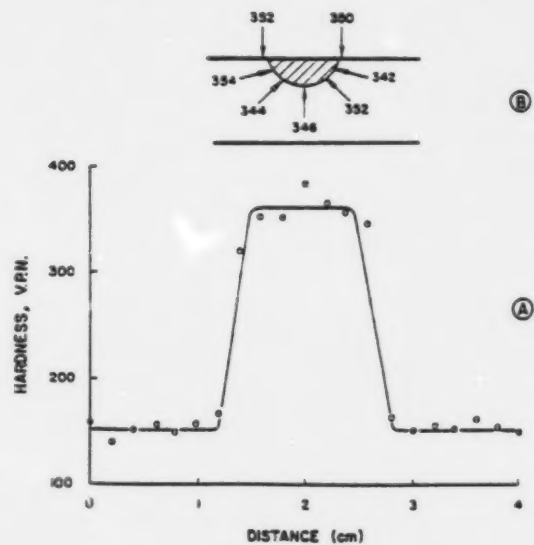
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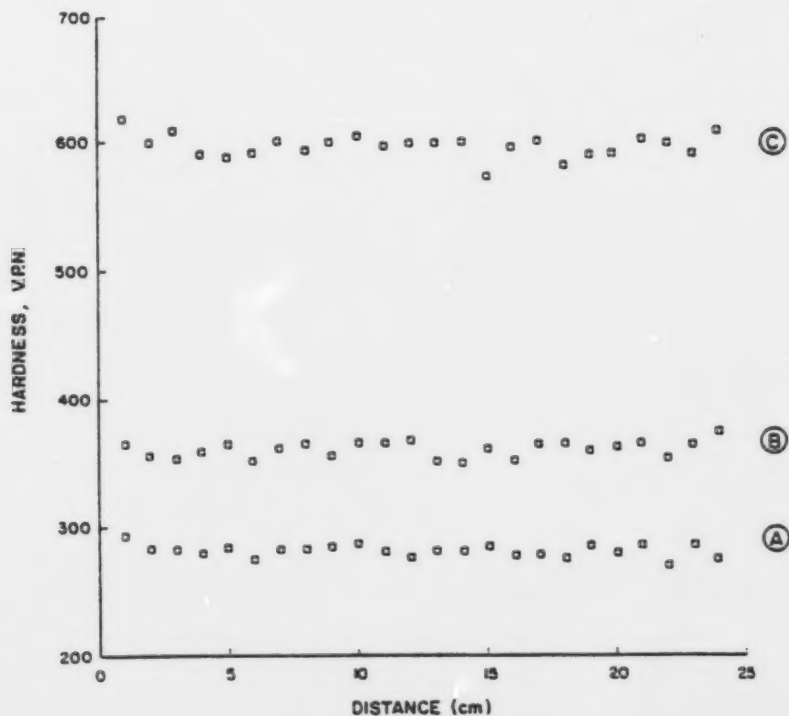
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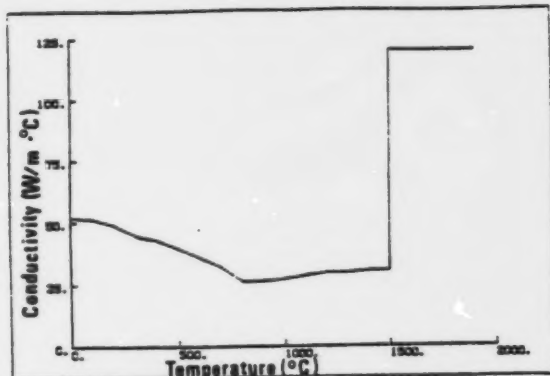
1. Characteristic hardness curve for a low carbon off-shore steel. Composition: 0.12C, 1.29Mn, 0.26Si, 0.15Cr, 0.14Ni, 0.10Mo, 0.053V, 0.16Cu, 0.030Nb, 0.008S, 0.007N, 0.015P.



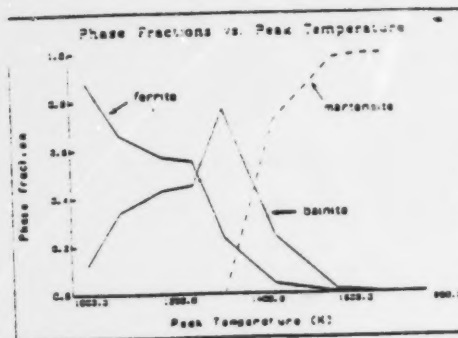
2. (A) Hardness traverse across the top of an autogenous electron beam weld and (B) hardness measured in the HAZ around the cross-sectional periphery.



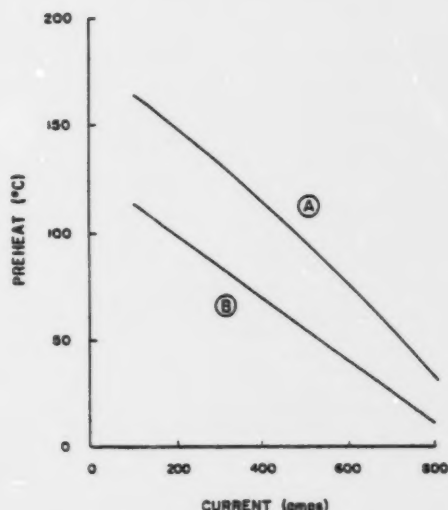
3. Hardness distribution along the length of autogenous electron beam welds. Note that the hardness dispersion is small.



4. Variation of thermal conductivity with temperature. Note that the thermal conductivity parameter assumed in the Adams approach of $22 \text{ W/m } ^\circ\text{C}$ is less than the real value at any temperature.



5. Microstructure distribution across a small bead-on-plate gas metal arc (GMA) weld. Heat Input: 0.21 kJ/mm ; base metal composition: 0.12C , 0.91Mn , 0.002P , 0.005S , 0.04Al , 0.021Nb , 0.011N .



6. Preheat to avoid cracking computations; submerged arc welding parameters: voltage-25V, welding speed-5mm/s; ambient temperature= -10°C ; base metal composition: 0.16C , 1.42Mn , 0.3Si , 0.02Ni , 0.03Cr , 0.07Cu , 0.012P , 0.001S , 0.02Nb , 0.006N , 0.03Al ; restraint conditions: workpiece thickness-25mm, restraint factor-400 N/mm^2 , joint stress concentration factor-2, material yield strength-500MPa, assumed workpiece size for the uniform preheat computation-1000mm X 4000mm; local preheat conditions: heater width-100mm, heater strength- 0.1 W/mm^2 , see reference 28 for more detail.

Carbon 0.1200	Ni 0.1350	U 0.0530	Nb 0.0390
Mn 1.2900	Cr 0.1500	B 0.0000	N 0.0070
Si 0.2700	Mo 0.1000	Cu 0.1600	S 0.0000

Arata 341.5544	Arata fm 0.7900
Beckert 370.1507	Yur. II fm 0.6316
Cottrell 374.6730	
Deuren 364.3141	Cool Time 3.5320
Suzuki 373.9686	
Terasaki 323.0116	
Yurioka I 300.0390	
Yurioka II 352.0842	

Cooling Time	0.0000
Voltage	34.0000
Amperage	200.0000
Efficiency	0.9500
Ambient Temp	20.0000
Thickness (mm)	25.0000
Welding Speed	9.3300

Press (esc) to switch between composition and weld parameters
 1EXIT 2 3 4 5 6 7 8 9RECALC 0

7. A convenient computer interface for weld hardness computations

AN ALGORITHM FOR MODELLING MICROSTRUCTURAL DEVELOPMENT IN WELD HEAT-AFFECTED ZONES (PART A) REACTION KINETICS

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Abstract—A computer algorithm originally developed for predicting the hardenability of low alloy steels has been adapted to forecast the microstructural development in weld heat-affected zones (HAZ). This algorithm simulates the kinetics of the decomposition of austenite to its various daughter products. When combined with a suitable model of the heat transfer in weld HAZ's, it provides a useful tool to predict the resultant microstructure. Thus, it allows one to optimize welding process parameters to achieve the best microstructure possible.

Résumé—Nous avons adapté à l'étude du développement microstructural dans des zones de soudure affectées par la température, un algorithme qui avait été développé au départ, sur ordinateur, pour prédire l'aptitude à la consolidation des aciers faiblement alliés. Cet algorithme simule la cinétique de la décomposition de l'austénite en ses différentes phases; combiné à un modèle adéquat du transfert de chaleur dans les zones de soudure, c'est un outil utile pour prédire la microstructure finale. Il nous permet ainsi d'optimiser les paramètres de la procédure de soudage pour réaliser la meilleure microstructure possible.

Zusammenfassung—Ein ursprünglich für die Voraussage der Härtung eines niedrig gekohlten Stahles entwickelter Computeralgorithmus wird so angepaßt, daß die Entwicklung der Mikrostruktur in wärmebeeinflussten Schweißzonen vorausgesagt werden kann. Dieser Algorithmus simuliert die Kinetik des Zerfalls des Austenits in seine verschiedenen Tochterprodukte. Der Algorithmus erweist sich als nützliches Hilfsmittel zur Voraussage der sich entwickelnden Mikrostruktur, wenn es mit einem geeigneten Modell des Wärmetransportes in den wärmebeeinflussten Schweißzonen kombiniert wird. Somit lassen sich die Schweißparameter im Hinblick auf die beste Mikrostruktur optimieren.

1. INTRODUCTION

The heat-affected zone (HAZ) which forms adjacent to the weld puddle in steels has both an intriguing metallurgical complexity and considerable commercial significance. It is the most common region of weld failure, and these failures are often related directly to the microstructure. When designing a weld joint, it is necessary to match the type of steel chosen with an appropriate welding process. One objective should be to avoid, to the extent possible, the formation of martensite. The welding parameters which have the greatest effect on microstructural development are the pre-heat practice, the heat input (welding current) and the weld travel rates. Computer algorithms have recently been developed [1-5] which can accurately simulate the temperature history of the weld puddle and its environs. It remains to couple this thermal record with an appropriate algorithm, sensitive to the steel chemistry, so that one can predict the microstructural development.

2. PREVIOUS WORK

The complexity of the local time-temperature histories, and the general nonlinearity of the kinetics of the metallurgical reactions makes an analytical prediction of HAZ microstructures intractable. It is, however, an interesting challenge for numerical modelling. Considerable effort has been put into numerical modelling of the welding process. It has been the subject of conference sessions [4, 5], but the main focus has been on the size and shape of the weld puddle, and on heat transfer from the weldment to the surrounding base metal. Publications modelling the development of the HAZ are relatively limited. There have been three basic approaches.

Coon and Watt [6] have shown that the hardenability algorithms developed by Kirkaldy *et al.* [7-11] can be used to forecast the resultant microstructure in the heat-affected zone. They [6] have further demonstrated that this type of algorithm can be used to isolate the individual effects of weld process pa-

rameters, or of metallurgical kinetic factors. In particular, they were able to use their algorithm to highlight the profound effect that austenite grain growth has on the HAZ microstructure. The general applicability of the Coon and Watt model is limited because of the use of a rather restrictive one-dimensional finite difference heat transfer algorithm. It is the purpose of this paper and the following paper to demonstrate that this basic algorithm, when combined with the more accurate three-dimensional finite element heat transfer program developed by Goldak *et al.* [1-3] can provide a powerful tool for weld process selection and control.

In the second type of method, several workers [12-14] have attempted to predict the hardness distribution through the HAZ without taking into account the phases present in the microstructure directly. The details of the calculations vary, but all are based on the hypothesis that the unknown hardness at some point in the HAZ can be predicted by matching that point with either a cooling rate at some temperature, or cooling time between two temperatures, on a sample piece of the same steel previously tested under known conditions. These known conditions are usually jominy test values or standard condition weld test beads. A numerical analysis of the heat flow from the weldment is then (usually) combined with an empirical matching of hardness values for a selected cooling time or cooling rate. There is no direct calculation of the metallurgical reaction rates. Often there is also the assumption that it is unnecessary to specifically use values like the peak temperature achieved, which affects the austenite grain size.

A more comprehensive approach has been developed by Ashby and Easterling *et al.* [15-17] to create microstructural HAZ diagrams in which the austenite grain size and the amount of martensite formed can be read directly off a map in cooling time- T_p space. Here the cooling time is the time to cool between 800 and 500 °C, and T_p is the peak temperature reached at a given point in the HAZ. The temperature distribution near the weld is assumed to obey a modified version of the analytical Rosenthal [18] equation. A weakness of the Rosenthal equations is that they assume that the thermal conductivity and specific heats of the materials are temperature independent. This is not so, and Moore *et al.* [3] have shown that ignoring this temperature dependence produces significant errors in the temperature distribution. In the Ion-Easterling-Ashby model [17] a "kinetic strength" of the heat cycle is calculated, which makes use of the comparative shape of the cooling curve, rather than the absolute prediction of temperature. The results have been correlated with actual welding experiments. A simplified kinetic equation is used to calculate the austenite grain growth. One of the most attractive features of the paper is that it does specifically include the effects of grain growth retarding nitrides and non-ferrous carbides. Approximate transformation rates for ferrite,

pearlite, bainite and martensite are calculated using the carbon equivalent index. This is somewhat crude, but the results have been correlated with actual welding experiments. These simplifications allow a fairly accurate prediction of the microstructure on a microcomputer. Creating a model which eliminates these approximations requires the use of either finite element or finite difference calculations, which is done better on a larger computer.

The objective of the present study is to describe an algorithm which will predict the extent of, and microstructure formed in, the HAZ of a welded steel for a wide range of chemical compositions as a function of the weld process input parameters. The approach has been as direct as possible. The algorithm through coupled calculations, keeps track of the metallurgical kinetics as they are driven by and contribute to the local temperature history, which is established by the weld heat input rates and the surrounding cold metal. Thus the algorithm comprises two parts: the generation of a heat transfer history, and the modelling of the metallurgical reactions. This paper will focus on the latter, making use of the hardenability algorithms developed by Kirkaldy and co-workers as the core.

3. MODELLING METALLURGICAL KINETICS

The heat-affected zone is a region varying between about 1 mm and 1 cm wide depending on welding conditions. It ranges from the line of greatest advance of the liquid-solid interface on its inner edge to the unaffected base material as its outer extreme. By definition, this reaches a temperature high enough to alter its microstructure and most of it becomes, at some time, at least partially austenitized. Compared with most metallurgical processes, the reaction times are short and the temperature changes severe. Suitable kinetic data for short term rapid heating are not available. In contrast, there is a wealth of data for a wide range of cooling rates because of its application in hardenability. Subject to these limitations, a metallurgical kinetics algorithm was developed to simulate the formation of austenite on heating, and its decomposition on cooling.

This part of the algorithm can be subdivided into two sections:

- (a) that which involves one time initialization of the parameters required for the general calculation, and
- (b) the time-temperature dependent reactions which are coupled with the heat transfer algorithm.

4. CREATING THE FRAMEWORK

Several important parameters involved in the metallurgical kinetic calculations are composition dependent. The first stage of the calculation is therefore to put in the compositions of the steel base metal and of the weld metal. With those one can then evaluate the appropriate physical constants.

To begin, the effect of composition of the equilibrium phase boundaries must be taken into account. Ideally these should be calculated from thermodynamic data in the manner of Hashiguchi *et al.* [11]. However, in some cases, simpler approaches are adequate.

For low alloy compositions, the liquidus and solidus lines can be regarded as a function of the carbon content only [19]. The presence of the transitory delta ferrite phase can be ignored if its effects on the heats of reaction are incorporated into the assumed liquid to austenite transformation. The error developed here is that a time delay for the delta to austenite reaction is overlooked. But this occurs in a region which will not be part of the heat affected zone. Thus, the effect of the time delay will, in general, be damped out by the time the heat release reaches the heat affected zone.

Since the weld metal is generally low carbon, we have chosen to approximate the liquidus as a linear function of the carbon content. For the solidus there are two choices. It can be assumed to be three straight lines jogged at the peritectic, or one straight line extrapolated back from higher carbon compositions to pure iron. Whichever version is chosen, the same amount of material is finally frozen, releasing the same amount of heat. The rate at which it is released depends on which alternative is chosen, but most of this difference is buffered out by the time the released heat passes into the HAZ.

The most accurate representation for the A_{e3} line is that of Kirkaldy and Baganis [10]. A linear series expansion for the activity coefficients of the alloying elements is coupled with their effect on the standard free energy changes to give a thermodynamically correct prediction of the effect (ΔT) of the total alloy addition on the A_{e3} temperature. This ΔT value is then added to an accurate empirical representation of the A_{e3} temperature for the alloy-free Fe-C system. While the formulae are intimidating at first reading, they are in fact quite simple to incorporate into a computer algorithm. A difficulty with this formulation is that the equations are difficult to invert for purposes of lever law calculations. An alternative is to therefore use [20]:

$$\begin{aligned} AE3(^{\circ}\text{C}) = & 912 - 203\sqrt{C} - 15.2\text{Ni} + 44.7\text{Si} \\ & + 104\text{V} + 31.5\text{Mo} + 13.1\text{W} \\ & - 30\text{Mn} - 11\text{Cr} - 20\text{Cu} \\ & + 700\text{P} + 400\text{Al} + 120\text{As} + 400\text{Ti} \quad (1) \end{aligned}$$

where the compositions are in wt%.

The eutectoid temperature is taken to be [21]

$$\begin{aligned} PS(^{\circ}\text{C}) = & 723 - 10.7\text{Mn} - 16.9\text{Ni} \\ & + 29\text{Si} + 16.9\text{Cr} + 290\text{As} + 6.4\text{W} \quad (2) \end{aligned}$$

The ferrite solubility line in the intercritical region is represented by

$$TF(^{\circ}\text{C}) = 912 - 8486C \quad (3)$$

The bainite start temperature, from [7] is

$$\begin{aligned} BS(^{\circ}\text{C}) = & 656 - 58C - 35\text{Mn} \\ & - 75\text{Si} - 15\text{Ni} - 34\text{Cr} - 41\text{Mo} \quad (4) \end{aligned}$$

and finally, the martensite start, from (21) becomes:

$$\begin{aligned} MS(^{\circ}\text{C}) = & 561 - 474C - 33\text{Mn} \\ & - 17\text{Ni} - 17\text{Cr} - 21\text{Mo}. \quad (5) \end{aligned}$$

Kirkaldy and Venugopalan [7] have shown that equations (2), (4) and (5) can be used to predict, with good accuracy, isothermal transformation diagrams for plain carbon and low alloy steels (hardenability steels) including boron steels.

Both the specific heat and thermal conductivity vary considerably as the temperature changes. For ferritic steels, the specific heat passes through a sharp peak at the Curie temperature [23]. This can be represented by two simple functions [6], for $T < 1000$ K (727 $^{\circ}\text{C}$)

$$C_p = \frac{1.117 \times 10^6}{(1010 - T)^2} + \frac{12622}{1010 - T} + 0.3485T + 355.6 \quad (6)$$

and for $T > 1000$ K

$$C_p = \frac{1.225 \times 10^6}{(T - 990)^4} + 0.1381T + 585.7 \quad (7)$$

where C_p is in J/kg K. This produces the variation shown in Fig. 1, which also represents an average empirical fit to the data in Ref. [23]. The common assumption that C_p is a constant value is clearly wrong. The use of a constant C_p for calculating 800–500 $^{\circ}\text{C}$ cooling times has been examined by Moore *et al.* [3], and it is found that considerable errors are developed which can only be compensated by assuming unrealistic thermal conductivity values.

The heats of reaction must be taken into account. This can be done by specifically including the heat

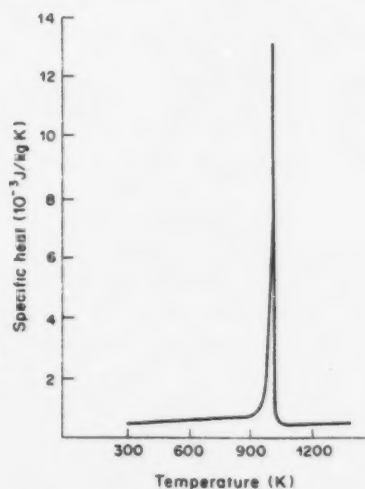


Fig. 1. Simulated variation of the specific heat with temperature.

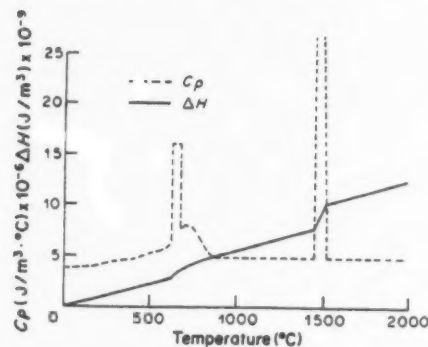


Fig. 2. The volumetric heat capacity and latent heats of fusion and transformation arranged for finite element computer implementation.

generated (or lost) as a term in the general energy balance equation for an element experiencing transient heat flow

$$q(\text{in}) - q(\text{out}) + q(\text{generated}) = \rho V C_p dT/dt \quad (8)$$

where ρ is the density and V is the volume of the element in question.

Alternatively, the heats of reaction can be incorporated indirectly in a modified specific heat function (3) as shown in Fig. 2, which includes the demagnetization peak at about 720°C.

The thermal conductivity varies as shown in Fig. 3. Here the conductivity in the liquid has been set at a relatively high value to take into account the convective stirring at the high velocities (~ 1 m/s) found in weld puddles [24].

5. MODELLING OF THE PHASE TRANSFORMATIONS

5.1. Melting and freezing of the weld puddle

The size and shape of the weld puddle is deter-

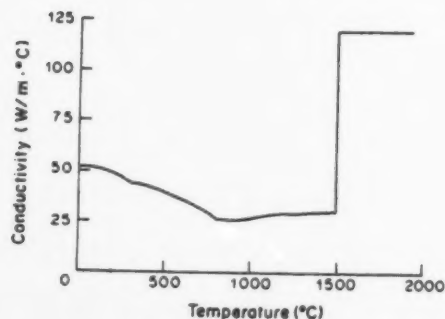


Fig. 3. The thermal conductivity-temperature relationship used in the finite element program. Note that a high conductivity in the molten region is used to simulate heat transfer by stirring.

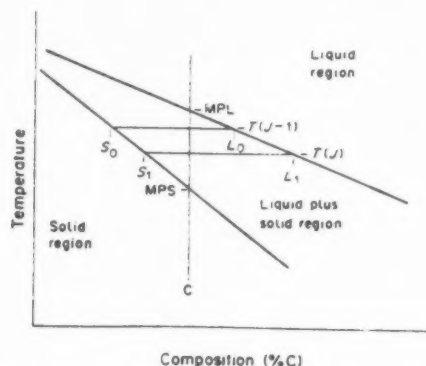


Fig. 4. Values of the parameters used in the solidification algorithm.

mined by the obvious parameters like the type of welding process, the plate thickness, heat input, and rate of weld travel. For modelling purposes, the effects of more subtle variables such as the heat flux distribution during welding must also be taken into account. The present study assumes a double ellipsoidal power density distribution for the heat source. The details of this model, developed by Goldak *et al.*, are published elsewhere [1]. The method has great flexibility and can accurately model processes ranging from shallow penetration arc welding processes to deep penetration electron beam welds.

To simulate freezing one essential assumption is made; that the kinetics of the freezing reactions are fast compared with the rate of heat removal. The rate of freezing is thus heat transfer controlled, and the corollary is that the amount of liquid or solid present will be given by the metallurgical equilibrium lever law calculation.

The freezing of the liquid steel in the fusion zone is based on a variable melting temperature between the liquidus and solidus lines previously mentioned. It is assumed that solidification can be represented by a single interface which moves across the freezing element through a series of incremental time steps. It is also assumed that all the material in the two-phase element is at the same temperature.

The amount of solid which freezes out during a given time step is calculated as follows; making reference to Fig. 4. At the beginning of the time increment the temperature is T_0 [or $T(J-1)$]. After convective heat loss to the next solid element, conductive gain from the upstream liquid element and the release of the heat of fusion ($f\Delta H$) from the freezing material, the temperature will drop to T_1 [or $T(J)$]. The amount of solid has increased from $(L_0 - C)/(L_0 - S_0)$ to $(L_1 - C)/(L_1 - S_1)$ where C is the overall carbon content of the weld metal. The freezing kinetics are thus determined by a balance between the external rate of heat transfer, and the heat released as determined by the lever law. The heat balance equation for a given time increment (J) can

be represented by

$$q(\text{in}) + f\Delta H - q(\text{out}) = \rho V C_p [T(J-1) - T(J)] \quad (9)$$

where $[T(J-1) - T(J)]$ is the change in temperature for the time increment, (i.e. $T_1 - T_0$) and f is the volume fraction of material frozen during the current time increment.

There are two unknown quantities in equation (9); f and $T(J)$. However, by making use of the lever law and the linear formulae for the liquidus and solidus lines, f can be restated as a quadratic function of $T(J)$ so that only one unknown remains.

The amount of solid formed in each time increment is added to the previous volume fraction of solid. When the temperature reaches MPS, this volume fraction reaches unity, the element has solidified and the freezing moves to the next upstream element. The C_p value used in equation (9) is a weighted average of the liquid and solid C_p values. In effect, it is assumed that with the passage of time, the interface moves from the downstream solid side of the element (when the temperature is at MPL in Fig. 4) to the originally liquid side of the element (when the temperature reaches MPS).

5.2. Austenitization and grain growth

On heating, austenitization can be expected to occur under near equilibrium conditions since superheating effects are small for most welding situations. In any event superheating effects are transitory throughout most of the HAZ and as long as the material does austenitize before grain growth begins (the carbide/nitride dissolution temperature in microalloy steels) then there is no effect on subsequent microstructure formation. This may not be entirely true in the intercritical region but this is expected to be a second order effect.

Newly formed austenite grains are assumed to be pinned by carbide/nitride precipitates (modern microalloy steels) until dissolution. A modified Ashby/Easterling [15] relationship is used to calculate the dissolution temperature

$$T_s = \frac{B}{A - \log(C_m^a C^b)} \quad (10)$$

where, A and B are constants that depend on the precipitate species; C and C_m are concentration of carbide (if carbide) and metal respectively (wt%); a and b are the stoichiometry constants for the precipitate in question.

After precipitate dissolution the austenite grains are assumed to expand according to the Ashby/Easterling [15] growth relationship

$$\frac{dg}{dt} = \frac{1}{2g} k \left[\exp\left(-\frac{Q}{RT}\right) \right] \quad (11)$$

where, g is the grain size (μm); k is the growth

constant ($\mu\text{m}^2/\text{s}$); Q is the activation energy for growth (kJ/mol); R is the gas constant (kJ/mol K).

Equation (10) represents the equilibrium precipitate solubility temperature, and takes no account of non-equilibrium effects due to the limited time available for precipitate dissolution. These may be significant for low energy welds where thermal cycles are rapid, and more important than superheating effects on phase transformations. It would be desirable to relate the austenite grain size to the instantaneous precipitate size and spacing during dissolution. This would require the assumption of an initial spectrum of precipitate sizes and spatial distribution. For the present, we simply assume that the precipitates all dissolve in a narrow temperature band.

In practice, temperature is a function of time $\Delta T(t)$ in a welding situation, and this expression must be integrated from the dissolution temperature around the thermal cycle to transformation completion.

The austenite grain size in the intercritical region and up to the dissolution temperature is assumed to be g_0 , the as-recrystallized size ($\sim 5 \mu\text{m}$ for most modern microalloy steels). The grain size in the fusion and mushy zone is complicated by melting. In addition this region is also complicated by chemical dilution from the filler material. There is no satisfactory grain size model for the fusion zone. However, it is known from experience that this region has a grain size similar to that of the coarse-grained HAZ immediately adjacent to the weld metal. In the absence of a better model, the fusion zone grain size is assigned the coarse-grained HAZ value.

5.3. Decomposition of austenite

Kirkaldy *et al.* [7-9] have developed a set of equations which model the austenite decomposition reactions for each of the diffusional products of austenite. These equations assume that a single continuous function can describe both the nucleation and subsequent growth for each of the daughter phases. For each reaction, the general reaction rate is characterized as

$$\frac{dX}{dt} = B(G, T) X^m (1 - X)^p \quad (12)$$

where X is the volume fraction of daughter product, B is an effective rate coefficient, G is the austenite grain size, and m and p are semiempirical coefficients set to less than one to assure convergence in a form that is derived from a point nucleation and impingement growth model [25].

The rate coefficient includes the effect of grain size on the density of eligible nucleation sites. It also includes the amount of austenite supercooling and the effect of alloying elements and temperature on diffusion.

Consider first the austenite to ferrite reaction. Above the AE3 line austenite is stable. As the temperature drops below AE3, ferrite begins to form.

Ferrite develops by nucleation at the austenite grain boundaries, and then growth into the austenite grains. The volume fraction of ferrite formed is thus a function of the nucleation rate, and the product of the area of the ferrite-austenite interface and its rate of advance. The last two factors in the general rate equation take into account the changing area of the austenite ferrite interface. The nucleation rate is primarily a function of the amount of supercooling below the AE3 line, and of the austenite grain size. A given reaction temperature affects both the diffusion rate of carbon and the degree of supercooling. For a given temperature, the degree of supercooling varies with alloy content because of the alloying elements' effect on the AE3 line. The alloys tend to be either austenite or ferrite stabilizers lowering or raising the equilibrium line respectively. Alloying additions can further inhibit transformation if the reaction requires their partitioning by phase boundary diffusion. Thus molybdenum, although it is a ferrite stabilizer, slows the reactions through its diffusional inhibition of the transformations.

Kirkaldy and Venugopalan [7] prescribe the austenite to ferrite reaction rate to be

$$\frac{dX}{dt} = \frac{2^{(G-1)/2} \Delta T^3 X^{2(1-X)^{-1}} (1-X)^{2X}}{\text{COM} \exp(-23,000/RT)} \quad (13)$$

where

$$\text{COM} = 59.6\% \text{Mn} + 1.45\% \text{Ni} + 67.7\% \text{Cr} + 244\% \text{Mo}$$

and dX/dt is in units of volume fraction per second; G is the ASTM grain size number for the austenite; $\Delta T = \text{AE3} - T$ is the amount of supercooling; X is the existing daughter product volume fraction, as defined below.

The denominator takes into account the diffusional resistance of the reaction and is developed from the general form

$$\frac{1}{D} = \frac{1}{D_c} + \sum_{i=1}^n \frac{k_i C_i}{D_i} \quad (13a)$$

where D is the effective diffusion coefficient calculated as the diffusion coefficient for carbon D_c modified by the presence of concentrations C_i of other alloying elements.

To get at a sense of the significance of each of these terms, consider that changing the grain size from 8 to 2 decreases the reaction rate by a factor of 8. Combining the interactive effects of composition and temperature, the value of the rate coefficient B [equation (12)] reaches a maximum of about 0.65 s^{-1} for 4140 steel at a temperature of about 865 K. For a highly weldable high Mn, low C pipeline steel, the maximum B is about 1.45 s^{-1} at 900 K. As the temperature decreases, the supercooling increases the rate as ΔT^3 but the diffusion rate slows as $\exp(-23,000/RT)$. The former term demonstrates that it is important to calculate AE3 accurately, particularly for slow cooling rates.

It is important to use the precise definition of X as given by Kirkaldy for equation (13). If one simply defines X as the volume fraction of ferrite then it is possible, using the kinetic equation (13) alone, to form more than the equilibrium amount of ferrite in the intercritical temperature region. This, and the relative change in the thermodynamic driving force for the reaction, are corrected by proposing a phantom reaction which can go to completion. The phantom reaction product is $X_f = X X_{fE}$ where X_{fE} is the equilibrium fraction of ferrite given by the lever law at that temperature. Thus in equation (13) we set $X = X_f/X_{fE}$. For temperatures below the eutectoid, and at times before the substantial production of a second daughter product, the eutectoid composition is used to find X_{fE} .

For pearlite formation, Kirkaldy prescribes a similar equation

$$\frac{dX}{dt} = \frac{2^{(G-1)/2} \Delta T D X^{2(1-X)^{-1}} (1-X)^{2X}}{1.79 + 5.42(\% \text{Cr} + \% \text{Mo} + 4\% \text{Mo}\% \text{Ni})} \quad (14)$$

where D is evaluated as

$$\frac{1}{D} = \frac{1}{\exp(-27,500/RT)} + \frac{0.01\% \text{C} + 0.52\% \text{Mo}}{\exp(-37,000/RT)}$$

and $\Delta T = PS - T$, the pearlite undercooling.

If some of the austenite has previously transformed to ferrite at the onset of pearlite formation, then the amount of unreacted austenite will be $(1 - X_f)$. As the pearlite forms, then the appropriate value for equation (14) is $X = X_p/(1 - X_{fE})$.

When the bainite start temperature is reached, it is assumed that pearlite growth degenerates to bainite formation. For the bainite reaction, we use

$$\frac{dX}{dt} = \frac{2^{(G-1)/2} (\Delta T)^2 \exp(-27,000/RT)}{(2.34 + 10.1\% \text{C} + 3.8\% \text{Cr} + 19\% \text{Mo}) 10^{-4} / (X, C_i)} \quad (15)$$

where

$$f(X, C_i) = \exp[X^2(1.9\% \text{C} + 2.5\% \text{Mn} + 0.9\% \text{Ni} + 1.7\% \text{Cr} + 4\% \text{Mo} - 2.6)]$$

and $\Delta T = BS - T$, the metastable bainite undercooling. It must be noted that $f(X, C_i)$ is set to 1 for all negative values of the exponent.

If pearlite exists when the bainite start temperature is crossed, then it is assumed that the existing pearlite-austenite interface continues to transform, but now yielding bainite. Then X in equation (15) is originally X_p . If no pearlite exists, then because the bainite reaction is sluggish, X is simply the fraction of bainite formed and it continues to transform until the remaining austenite is consumed or the MS temperature is reached.

It is assumed that whatever austenite has not decomposed at *MS* will become martensite on further cooling.

It would be a simple matter to develop an equation for retained austenite as a function of carbon content. However, this constituent becomes a significant volume fraction only at medium to high carbon contents where the martensite formed is brittle. For the purposes of weld heat-affected zones, the object is to find the conditions that will avoid the development of brittle regions. Thus the presence of retained austenite is regarded as incidental.

6. DISCUSSION

The algorithms for the decomposition of austenite developed by Kirkaldy and co-workers have been combined with a finite element heat transfer model to predict the HAZ microstructure. The heat transfer part of the algorithm has been shown to be very accurate, possibly better than any of the current experimental methods than can be used to evaluate it [1]. The form of the austenite decomposition equation has its basis in the theory of reaction kinetics. The empirical factors used have been massaged over a period of 20 years to produce a good fit to the *IT* and *CCT* diagrams of over 200 different steel compositions [7]. The great advantage of the method is that one algorithm, once developed, can be applied to a broad range of steel compositions by simply entering the steel chemistry as input data.

The reaction kinetic arguments on which the algorithm are based are not universally accepted. In particular, Hawbolt *et al.* [26, 27] have argued that it is necessary to separate the nucleation kinetics from the growth rate processes, with the additivity principle only applicable to the latter. The result is that an incubation time should be included before growth equations with a form similar to equations (12–15) are applied. Their data and arguments are persuasive. For an individual steel for which there is known data, their formulae will give a more accurate result. But data in this form are at present limited to very few alloys. More importantly, there is at present no general chemistry dependence developed for the range of alloys covered by Kirkaldy's data. Under these circumstances, we conclude that the present algorithm is the only choice to predict the microstructure directly for a range of steel compositions. Based on its ability to predict *IT* diagrams [7], it should be more than adequate for HAZ use.

In the paper which follows, the details of the heat transfer part of the algorithm will be explained, and experience in using the algorithm as a predictive tool elucidated.

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COUPLED TRANSIENT HEAT TRANSFER—MICROSTRUCTURE WELD COMPUTATIONS (PART B)

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Abstract—The Watt/Coon algorithm put forward in Part A is coupled to a transient finite element heat transfer analysis for computing the microstructure as a function of space and time (x, y, z, t) in the heat-affected zone (HAZ) of low alloy steel welds. The input data are the composition, the thermal properties, the initial microstructure and the initial temperature of the base material, the geometry of the joint, the convective and radiative boundary conditions, and the shape and power density distribution of the heat source. Computed prior austenite grain size and residual microstructures (ferrite, pearlite, bainite, and martensite fractions) for a bead-on-plate low carbon steel weld are compared against measured values to evaluate the approach. Computer generated contour representations are presented to map microstructural fields for easy interpretation. Transient microstructural changes are included to demonstrate the capability of the system. As far as these authors know the Watt/Coon algorithm is the first model capable of predicting transient microstructural changes. Combined with FEM heat transfer analysis it is shown that this represents a very powerful system.

Résumé—L'algorithme de Watt de Coon présenté dans la partie A est associé à une analyse aux éléments finis du transfert de chaleur transitoire, dans le but de calculer sur ordinateur la microstructure en fonction de l'espace et du temps (x, y, z, t) dans la zone affectée par la température de soudures dans les aciers faiblement alliés. Les données de départ sont la composition, les propriétés thermiques, la microstructure initiale et la température initiale du matériau d'origine, la géométrie de la liaison, les conditions aux limites de convection et de radiation, ainsi que la forme et la répartition de la densité de puissance de la source de chaleur. Pour tester cette approche, nous avons comparé à l'expérience la taille des grains d'austénite et les microstructures résiduelles (ferrite, perlite, bainite et martensite) calculées antérieurement sur ordinateur. Pour faciliter l'interprétation, nous présentons les figures des contours générés à l'ordinateur pour dresser une carte des champs de microstructures. Les modifications transitoires de microstructure sont incluses pour démontrer l'efficacité du système. À notre connaissance, l'algorithme de Watt et Coon est le premier modèle capable de prédire les modifications transitoires de microstructure. Combiné à une analyse aux éléments finis de transfert de charge, il constitue un système très puissant.

Zusammenfassung—Der im Teil A behandelte Watt/Cohn-Algorithmus wird an eine Finite-Element-Analyse des transienten Wärmetransportes gekoppelt, um die Mikrostruktur in Abhängigkeit von Raum und Zeit (x, y, z, t) in der wärmebeeinflussten Zone von Schweißnähten in niedrig gekohlten Stählen zu berechnen. Die dabei einzugebenden Daten sind Zusammensetzung, thermische Eigenschaften, anfängliche Mikrostruktur und Temperatur des Grundmaterials, die Geometrie der Schweißverbindung, die konvektiven und radiativen Randwertbedingungen und Form und Energiedichteverteilung der Wärmequelle. Um diesen Ansatz zu überprüfen, werden die für eine Schweißraupe auf niedrig gekohltem Stahl berechneten Austenitkorngrößen und die restliche Mikrostruktur (Ferrit, Perlit, Bainit und Martensitanteile) mit gemessenen Werten verglichen. Mit Computer-erzeugten Konturkarten werden die Bereiche leichter Interpretation dargestellt. Die Veränderungen der Mikrostruktur während der Transienten sind mit aufgenommen, damit die Möglichkeiten dieses Verfahrens dargestellt werden. Nach unserer Kenntnis ist der Watt/Cohn-Algorithmus das erste Modell, welches die ablaufenden mikrostrukturellen Änderungen voraussagen kann. Kombiniert mit einer FEM-Analyse des Wärmeüberganges stellt es sich sogar als ein sehr fähiges System heraus.

INTRODUCTION

One of the primary goals of computational weld mechanics is to establish a comprehensive system for analysing the thermo-mechanical changes that occur during the welding process. Such an analysis is basic to understanding the mechanics that control the appearance of cracks that form in the HAZ as the

weld cools, and the crack free mechanical properties of the joint as a whole. There is a considerable volume of literature describing finite element modelling for the purpose of computing transient temperature, displacement and stress fields (x, y, z, t) in various situations [2-4]. However, until now these have not been coupled to reaction kinetic theories to compute microstructural changes.

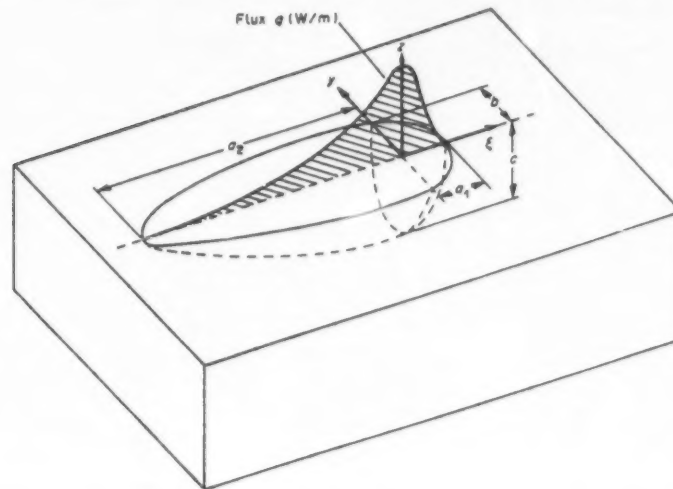


Fig. 1. Double ellipsoid with superimposed Gaussian energy distribution used to model a welding heat source [2].

The need to integrate microstructural models into the system is twofold. It is apparent that the mechanical properties of the HAZ depends on residual microstructure (daughter products as a result of austenite decomposition) and there is a need to control the size, shape and distribution of HAZ phases. However, over and above this there is a need to track the microstructure. Accurate finite element computations require thermal and mechanical property input over the entire thermal cycle. It is apparent that tracking microstructural changes and eventually feeding these back into the computations is a key component of such analyses.

In this investigation the reaction kinetics algorithm put forward by Watt *et al.* [1] is coupled to the FEM heat transfer models established by Goldak and Associates [2] to predict HAZ microstructural changes. The system is supported by comparing microstructural computations to some of the HAZ experimental measurements of Ion for a low carbon microalloy structural steel [5]. Microstructure contour representation is proposed for easy interpretation of the results. To demonstrate the capacity and flexibility of the system, transient microstructural changes are tracked throughout a weld cycle for various positions in the HAZ.

FINITE ELEMENT MODEL

The heat source and workpiece arrangement used for the finite element computations of a bead-on plate weld are shown in Fig. 1. The heat source is represented by a double ellipsoid configuration that is roughly the shape of the weld pool. A Gaussian energy distribution is imposed on the ellipsoid in all three dimensions. It is a maximum immediately

beneath the heat source and decays to the ellipsoid boundaries. In the absence of more detailed knowledge, a Gaussian energy distribution is said to approximate the complex heating effect due to the magnetohydrodynamic interaction of the arc and weld pool. Such a model has been used previously with considerable success [6, 7].

The size of the weld pool is estimated for any general welding situation with a method first suggested by Christensen [8]. The heat source is then arbitrarily set to a size that is 5–10% smaller than the weld pool. By so doing some weld pool superheating appears which is known to be the case in practice. As the superheat dissipates the weld pool melts out to the proper dimensions. If the superheat temperature exceeds 2500 °C (based on experimental measurements [8]) or if the melt out dimensions are not consistent with the Christensen or measured values, the ellipsoid is adjusted and the computations are redone. While this may seem somewhat arbitrary, it has been shown that accurate thermal fields are computed with this procedure. It is these authors' view that this is the best that can be done since the detailed magnetohydrodynamics of the arc and weld pool are not well enough understood to be modelled with sufficient confidence at this time.

In addition to the heat source model a heat flow kinematic model must be selected. In Refs [2–4] heat flow is assumed to be constrained to a plane perpendicular to the direction of heat source motion. It is argued that this constraint is necessary to keep computing time and costs within reason. At the same time thermal gradients in the cross-sectional plane are usually much greater than they are along the weld and the error caused by making such an assumption is said to be small. While this may be true in most

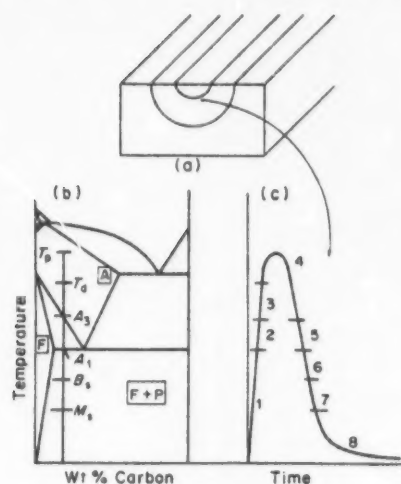


Fig. 2. (a) Schematic cross-section of a bead-on-plate weld identifying a point in the HAZ for study, (b) Fe-C phase diagram identifying the cooling path and critical temperatures, (c) thermal cycle identifying the regions that must be considered when implementing the microstructure algorithm.

cases it is widely recognized that a full three-dimensional analysis would be preferable. Recently, three-dimensional automatic adaptive mesh grading algorithms have been added to these authors' system that permits full three-dimensional computations [9].

Temperature dependent thermal properties, for low alloy steels are built into the system as are convective/radiative boundary conditions [7]. All nodes are initialized to the preheat temperature. Joint and workpiece geometry is automatically taken into account by meshing to the workpiece boundaries. FEM calculation systems are well known and in

particular FEM applied to the welding process is well documented. Details of the system used are contained in Refs [2, 6, 7].

IMPLEMENTING THE MICROSTRUCTURE ALGORITHM

The method of implementing the microstructure algorithm is best described with reference to the diagrams in Fig. 2. Point 1 is an arbitrary HAZ position. The cooling path and critical temperatures are represented by the line path drawn on the Fe-C phase diagram in Fig. 2(b). The corresponding thermal cycle is shown in Fig. 2(c) for a typical HAZ position [Fig. 2(a)].

In practice the thermal cycle is generated by FEM for any point in the fusion zone or HAZ. The microstructure algorithm tracks the thermal cycle, and structural changes are computed according to the relationships contained in Table 1. Thermal properties consistent with the structure computed can be returned to the FEM analysis during each time step. A description of the relationships and thermal properties used in this investigation are contained in the accompanying paper (Part A—Watt *et al.*) [1].

Equilibrium is assumed on heating and structural changes are computed according to the phase diagram [Fig. 2(c), Regions 1, 2 and 3]. Microstructure kinetics begin when the carbide and nitride precipitates that pin the austenite grains dissolve (Region 4). In the HAZ austenite grains grow until they decompose on cooling. An initial recrystallized grain size must be assigned which is typically set to 5–10 μm for most modern microalloy steels.

Ferrite forms in region 5 and continues into Region 6 until pearlite begins to form. This is consistent with CCT (continuous cooling transformation) principles.

Table 1. Microstructure calculation methods and constraints^{a,b}

Region	Relationships	Comments
I (RT to PS)	$X_F = (C_F - C)C_F$	Equilibrium assumed
II (PS to A_1)	$X_P = 1 - X_F$	PS obtained from equation (2)
III (A_1 to TS)	$X'_F = (C_A - C)C_A - C_1$	C_A obtained from equation (1)
IV (TS to A_1)	$X_A = 1 - X'_F$	C_1 obtained from equation (3)
	$X_A = 1$, $G = G_0$	TS obtained from equation (10)
	$X_A = 1$	
V (A_1 to PS)	$G = G_0 + \Sigma \Delta G$	ΔG obtained from equation (11)
	$X_F = \Sigma \Delta X_F$	ΔX_F obtained from equation (13)
	$X_A = 1 - X_F$	
VI (PS to BS)	$X'_F = X_F$ (Region V) + X_F	$\Delta X'_F$ obtained from equation (13)
	$X_P = \Sigma \Delta X_P$	ΔX_P obtained from equation (14)
		If $X_P > 0.01$, stop ΔX_F
	$X_A = 1 - X'_F - X_P$	BS obtained from equation (4)
VII (BS to MS)	$X'_F = X'_F$ (Region VI)	MS obtained from equation (5)
	$X_P = X_P$ (Region VI)	
	$X_B = \Sigma \Delta X_B$	ΔX_B obtained from equation (15)
		(Initial $X_B = X_P$)
VIII (MS to RT)	$X_A = 1 - X'_F - X_P - X_B$	
	$X'_F = X'_F$ (Region VII)	
	$X_P = X_P$ (Region VII)	
	$X_B = X_B$ (Region VII)	
	$X_M = X_A$ (region VII)	Austenite decomposes to Martensite at MS

^aFor explanation of regions see Fig. 2(c).

^bEquations are to be found in accompanying paper (Watt *et al.*) [1].

In practice the ferrite algorithm is stopped when the pearlite content reaches $x_p = 0.01$.

Pearlite and ferrite form in Region 6 until the bainite start temperature is reached (Region 7). The bainite algorithm is then activated with the constraint that it is initialized to a "ghost fraction" equal to the amount of pearlite from Region 6. The rationale for this is contained in Kirkaldy's original reaction kinetics presentation [10]. Essentially bainite nucleation occurs at pearlite sites and, therefore, the pearlite appears as bainite to the reaction kinetics governing the transformation. Bainite formation continues until the martensite start temperature (Region 8) where it is assumed that all remaining austenite decomposes to martensite.

If the maximum temperature of the thermal cycle exceeds the solidus, the microstructure algorithm must be adjusted for melting. Essentially equilibrium concepts are applied to this region. It is, of course, recognized that supercooling, nonequilibrium solidification and other such phenomena occur and, in principle, can be incorporated in the algorithm. For problems such as "hot cracking" these undoubtedly play an important role and will have to be taken into account. However, the situation is complex for the welding process because of compositional changes, among other things. Since this study is primarily concerned with the heat-affected zone, applying refined non-equilibrium concepts to the fusion and two phase regions is left to further study.

In this study when a thermal cycle "peaks out" between the solidus and liquidus, the equilibrium amounts of solid and liquid are computed. The solid is assigned the base metal composition while the composition of the liquid metal is adjusted for dilution. Dilution occurs if the composition of the filler metal is different than that of the base material. The term dilution is applied because the alloying content of the filler wire is almost always less than the alloying content of the workpiece. Dilution values (fraction base metal fused into the molten pool) are available for most welding processes [11].

In addition to adjusting the algorithm for composition when it is applied above the solidus, Ashby's grain growth kinetics no longer applies [1]. It is not yet possible to compute the grain size of the fusion and two-phase (S-L) regions. However, it is known that the grain sizes in these regions are large—at least as large as the coarse grained region of the HAZ immediately adjacent to the FZ. In view of this the grain size in the FZ is arbitrarily set equal to the maximum grain size of the HAZ. Undoubtedly this can be refined with further work.

The intercritical area (between PS and A₁) is yet another region that requires special explanation. Equilibrium is assumed on heating which is not justified, in principle, because carbon diffusion is limited in short time weld thermal cycles. However, transformation kinetics is not well known and in any event the consequences of assuming equilibrium on

heating are physically unimportant. For those regions where the thermal cycle passes completely through the intercritical region, subsequent transformations eliminate the history of this region. If the thermal cycle is closely coupled to the microstructure (i.e. thermal properties are folded back into the FEM thermal history computations) some effect on the thermal cycle can be expected. However, this too is not very significant since the most important microstructural changes occur on cooling. Certainly the computations are suspect in those regions where the peak temperature ends up between PS and A₁. Equilibrium on heating overestimates the austenite formed and, in turn, the decomposition products are overestimated in this situation. However, since the properties of the intercritical HAZ region are better than those of the base metal, it is rarely an area of concern.

In summary then, these authors contend that assuming equilibrium on heating does not lead to any great difficulty in interpreting microstructural computations in the HAZ. On the other hand when superheating ferrite austenite kinetics and non-equilibrium solidification effects are better understood adding them to the algorithm is recommended. On cooling in the solid state Kirkaldy reaction kinetics is applied to track the decomposition of austenite.

CODING PRECAUTIONS

Coding the algorithm is straightforward in principle but is relatively complex in practice when coupled to FEM analysis. Relatively large time steps (0.05 s or larger) are suitable for the FEM analysis because the temperature gradient changes slowly. On the other hand time steps as small as 10^{-4} s are required to integrate the decomposition equations. Dealing with these different time scales requires considerable care in the numerical analysis and programming. This problem is especially difficult near region boundaries (see Fig. 2).

Added to this is the problem of numerically integrating the sigmoidal decomposition relationships along a thermal path. Because the reaction rate varies dramatically during transformation a simple Euler integration technique is inefficient over much of the cycle. Consequently the algorithm can very quickly become CPU intensive and costly. These authors suggest automatic error checking, adaptive ODE integration routines for solving these equations more efficiently.

A COMPARISON OF COMPUTED AND MEASURED RESULTS

To test the validity of the system the computed microstructural distribution in the HAZ of a low carbon microalloy bead on plate steel weld is compared with the measured results of Ion [5]. Such

Table 2. Base metal composition⁽¹⁾ and operating parameters⁽²⁾ for the microalloy steel weld analysed

(1)	C-0.12 Nb-0.021	Si-0.16 N-0.011	Mn-0.91	P-0.002	S-0.005	Al-0.04
(2)	Bead on plate weld; process—gas metal arc, gross heat input—0.21 kJ/mm, efficiency—0.75, plate thickness—12.7 mm					

measurements are very difficult in practice because of the small size of the HAZ. Some of the best measurements available are those of Ion. The base metal composition and the welding parameters of the weld studied are given in Table 2.

To compute the prior austenite grain size distribution in the HAZ, it is first of all necessary to assign the as recrystallized grain size ($g_0 = 10 \mu\text{m}$), the activation energy ($Q_s = 241.2 \text{ kJ/mol}$) and the growth constant [equation (11), Part A]. The activation energy is taken from the work of Easterling and Ashby [12] but a value for the kinetic growth constant is not available. However, by comparing computed and measured grain sizes it soon became apparent that a value of $k = 7 \times 10^5 \text{ mm}^2 \text{ s}^{-1}$ was appropriate for this steel. This conclusion is supported by two observations. First there is excellent agreement between the measured and computed grain size values when $k = 7 \times 10^5 \text{ mm}^2 \text{ s}^{-1}$ is used (Fig. 3). While this particular weld (heat input = 0.21 kJ/mm) is offered for presentation, similar agreement is experienced for three other bead-on-plate heat input ranges (0.2–1.1 kJ/mm). Secondly there is good agreement between measured and computed values throughout the HAZ i.e. the distribution match (grain size vs peak temperature) is good. This lends support to the values for both kinetic constants (activation energy and growth constant) used in these computations.

In addition to the grain growth constants, the dissolution kinetic parameters must be specified. Since the austenite grains are stabilized by NbC in this particular case, the constants are $A = 3.11$ and

$B = 7520$ (equation (11) [1]). These are the constants suggested by Easterling–Ashby [12] based on the original work of Nordberg and Aronsson [13]. Austenite grain growth is started at the point of complete carbide dissolution. This can be questioned because presumably some growth can occur before this time i.e. during the dissolution process. However, the dissolution range is relatively narrow and in any event most of the growth occurs at higher temperatures. Therefore, ignoring growth during dissolution is justified.

The second measurement reported by Ion [5] is the fraction martensite distribution in the HAZ as shown in Fig. 4. In this case there would seem to be considerable divergence between the measured and computed values. The measurements suggest a continuous decrease in the martensite fraction from the FZ/HAZ boundary to the HAZ/base metal boundary. The computations, on the other hand suggest a sharp decrease in the martensite fraction at approximately 1400 K (1137 °C).

Before presenting arguments to clarify this disparity it is useful to examine the hardness distribution in the HAZ as shown in Fig. 5. A rule of mixtures is used to generate the hardness values from the microstructural computations. The component relationships used in the rule of mixtures computations are taken from the work of Maynier *et al.* [14]:

$$H_M = 127 + 949(C) + 27(\text{Si}) \\ + 11(\text{Mn}) + 8(\text{Ni}) + 16(\text{Cr}) + 21(\log t)$$

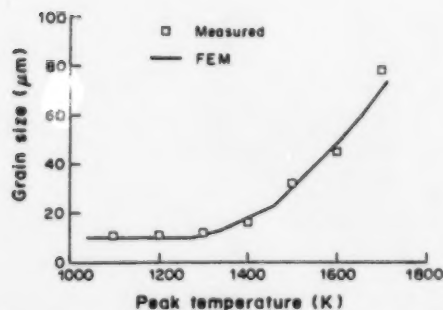


Fig. 3. HAZ grain size distribution (i.e. grain size vs peak temperature) for a bead-on-plate microalloy steel weld. Base plate composition and welding parameters contained in Table 2.

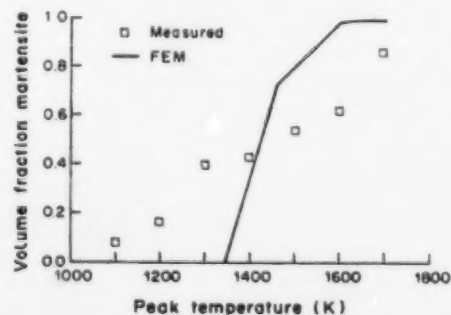


Fig. 4. HAZ fraction martensite distribution (i.e. fraction martensite vs peak temperature) for a bead-on-plate microalloy steel weld. Base plate composition and welding parameters contained in Table 2.

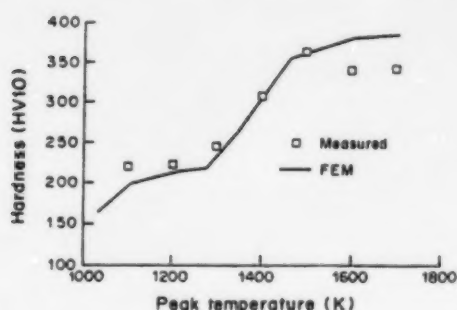


Fig. 5. HAZ zone hardness distribution (i.e. hardness vs peak temperature) for a bead-on plate microalloy steel weld. Base metal composition and welding parameters contained in Table 2.

$$H_b = -323 + 185(C) + 330(\text{Si}) + 153(\text{Mn}) \\ + 65(\text{Ni}) + 144(\text{Cr}) + 191(\text{Mo}) \\ + [89 + 53(C) - 55(\text{Si}) - 22(\text{Mn}) \\ - 10(\text{Ni}) - 20(\text{Cr}) - 33(\text{Mo})] \log V$$

$$H_{fp} = 42 + 223(C) + 53(\text{Si}) + 30(\text{Mn}) \\ + 12.6(\text{Ni}) + 7(\text{Cr}) + 19(\text{Mo}) \\ + [10 - 19(\text{Si}) + 4(\text{Ni}) + 8(\text{Cr}) \\ + 130(V)] \log V$$

where

H_M = martensite hardness (VPN)

H_b = bainite hardness (VPN)

H_{fp} = ferrite-pearlite hardness (VPN)

V = cooling rate at 700°C (°C/h)

log = logarithm to base 10.

It is important to recognize the limits of these equations: 0.1 wt% < C < 0.5 wt%, Si < 1 wt%, Mn < 2 wt%, Ni < 4 wt%, Cr < 3 wt%, Mo < 1 wt%, V < 0.2 wt%, Cu < 0.5 wt%, Mn + Ni + Mo < 5 wt%, and 0.01 wt% < Al < 0.05 wt%. They can only be applied to low carbon steels with reservations, and the microalloy elements Nb, Ti, Zr and B are not taken into account.

A comparison of the computed and measured hardness distribution is shown in Fig. 5. It is evident that there is good agreement. At the same time there is a relatively sharp change in the hardness distribution where the peak temperature is approximately 1400 K. Since hardness is very sensitive to the martensite fraction, this would imply that the martensite fraction changes rapidly at this same position in the HAZ contrary to the measurements in Fig. 4. A rapid change in martensite implies a considerable change in hardenability. This, in turn, is caused by grain growth which has a surprisingly strong effect on the decomposition relationships (equations (13–15) [1]).

In general terms the agreement achieved between the computed and measured distributions is consid-

ered excellent in spite of the disparity shown in Fig. 4. In view of the foregoing arguments and the results shown in Fig. 5, the cause of the disparity in Fig. 5 (measurements or computations) is matter for debate. The measurements are very difficult because of the small size of the HAZ and yet they are well done (the best available). In addition, the computations rely on considerable data that may or may not be entirely reliable.

CONTOUR REPRESENTATIONS

One of the advantages of an integrated FEM thermomicrostructure system is that contour representations that map constant phase fractions of microstructures are possible. Such a representation is shown for the temperature and austenite fields in Fig. 6. The term quasi-stationary was coined by Rosenthal [15] to describe the fact that they are stationary with respect to the heat source but are moving along the workpiece at the welding speed. An austenite zone around the heat source is expected. If the system were in equilibrium in both heating and cooling the shape of the temperature and austenite isomicrostructure contours would be the same. However, on cooling austenite persists to temperatures well below the equilibrium region. This has the effect of elongating the austenite isomicrostructure contours on the cooling side of the heat source which is clearly shown in Fig. 6.

Contours of residual ferrite and bainite cross-sectional contours are shown in Figs 7 and 8. In Fig. 7, the ferrite fraction near the fusion zone boundary is small (martensite is the principle constituent in this area) and it increases to the equilibrium value of 0.87 as the HAZ boundary is approached. The discontinuity in some of the contours is an artifact of the plotting system. The FEM elements developed by McDill [9] sometimes contain sub-elements which are ignored by the plotting routine. Both the automatic plotting routine and the McDill elements are under development at this point and the problem will eventually disappear. However, there is no question that the contours generally represent the correct microstructure fraction and interpretation is not difficult.

The bainite fraction shown in Fig. 8 is zero near the FZ/HAZ boundary and near the HAZ/base metal boundary. There is an increase in bainite content in the central regions of the HAZ. This is clearly shown in Fig. 9. At any point the phase fraction must sum to 1. At the FZ/HAZ boundary the balance is martensite while it is ferrite at the HAZ/base metal boundary. Once again there are interpolation anomalies with the automatic plotting routine but these are not serious enough to cause interpretation difficulties. It is curious that there is no pearlite in the HAZ of this particular weld. This is, perhaps, not too surprising in view of the relatively rapid cooling (800–500°C cooling time of approx. 1 s) and the fact

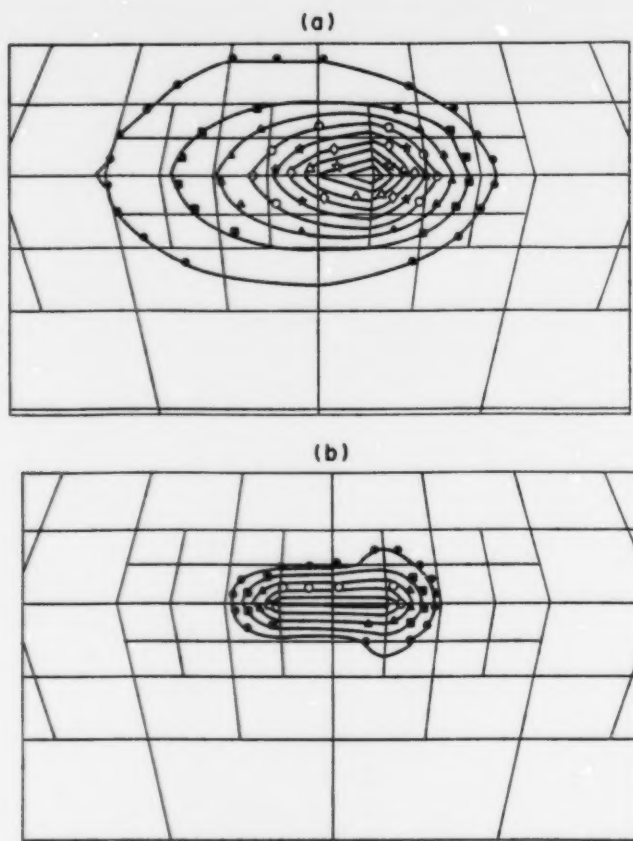


Fig. 6. Temperature isotherms (A) and corresponding austenite isomicrostructure contours (B).

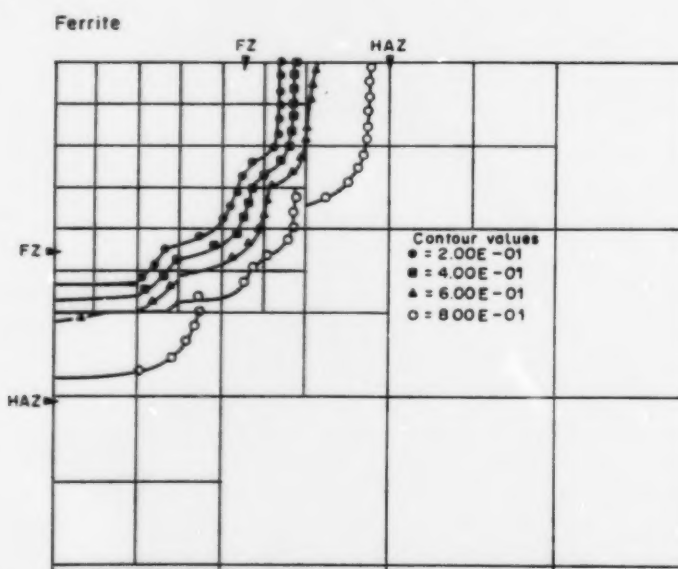


Fig. 7. Isoferrite contours mapped on the HAZ cross-section of the bead-on-plate weld. Base metal composition and welding parameters given in Table 2. Note: fraction ferrite code: A = 0.2, B = 0.4, C = 0.6, D = 0.8.

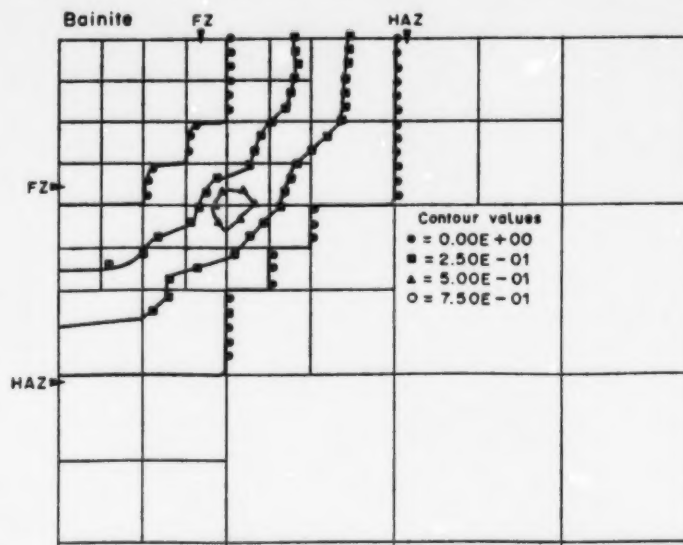


Fig. 8. Isobainite contours mapped on the HAZ of the bead-on-plate weld. Base metal composition and welding parameters given in Table 2. Note: fraction bainite code: A = 0, B = 0.25, C = 0.50, D = 0.75.

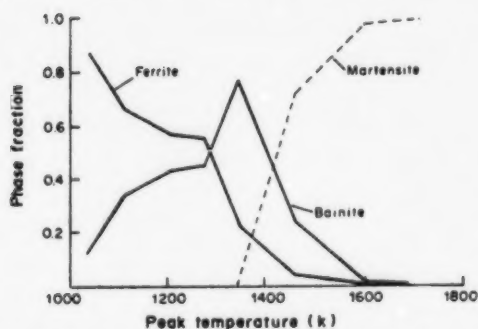


Fig. 9. Variation of ferrite, bainite and martensite throughout the HAZ of the bead-on-plate weld. Base metal composition and welding parameters contained in Table 2.

that the equilibrium value of pearlite is small in any event (approx. 0.12).

TRANSIENT MICROSTRUCTURAL CHANGES

Apart from computing the final (residual) microstructures (prior austenite grain size, fractions ferrite, pearlite, bainite and martensite) the computation of transient structural changes is an important development. The FZ and HAZ boundaries and two nodes (designated 98 and 102) are shown in Fig. 10. The computed thermal cycles for these two nodes are shown in Fig. 11. Node 102 is close to the FZ/HAZ boundary and has a relatively high peak temperature

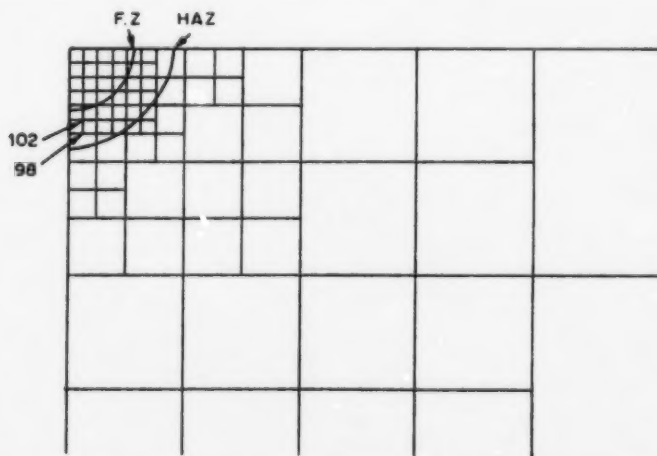


Fig. 10. Cross-section showing the position of the fusion zone boundary (corresponds to a maximum temperature of $T = 1510^{\circ}\text{C}$) and the HAZ boundary (corresponds to a temperature of $PS = 718^{\circ}\text{C}$ for this steel). Base metal composition and welding parameters contained in Table 2.

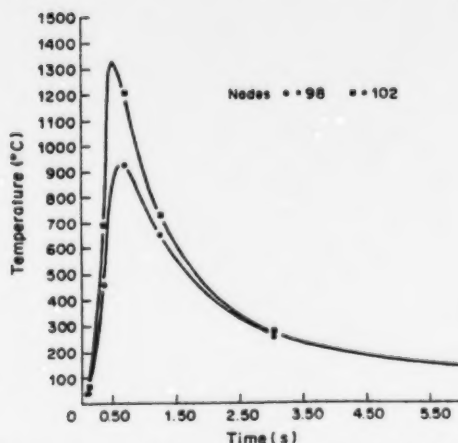


Fig. 11. Computed thermal cycles for nodes 98 and 102 shown in Fig. 10. Welding parameters contained in Table 2.

($T_p = 1350^\circ\text{C}$). On the other hand node 98 is central to the HAZ and has a lower peak temperature ($T_p = 950^\circ\text{C}$). As a consequence the grain growth and hardenability of these two positions is quite different. The transient microstructural changes for node 98 are given in Fig. 12. Initially the ferrite fraction is at the equilibrium value of 0.87. This persists until the temperature reaches PS (718°C in this case) when ferrite-pearlite disappears and austenite is formed. Eventually the austenite gives way to ferrite and bainite as the weld cools. It is interesting to note how quickly the austenite forms (between PS and A_1) and how quickly it decomposes in a welding situation. Decomposition occurs in approximately 0.5 s for this low heat, low carbon microalloy welding situation. By displaying the transient microstructural behavior

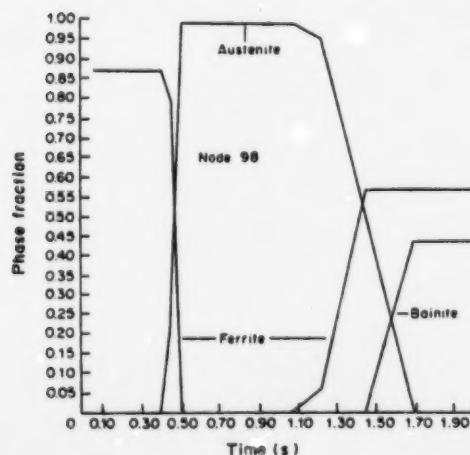


Fig. 12. Transient microstructural changes for node 98—see Fig. 10 for position. Welding conditions are contained in Table 2.

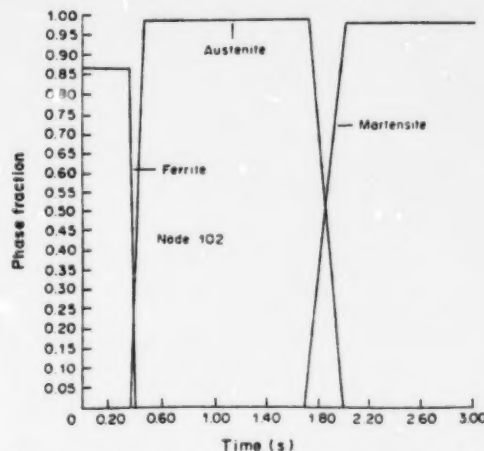


Fig. 13. Transient microstructural changes for node 102—see Fig. 10 for position. Welding conditions are contained in Table 2.

in the HAZ, a much better picture of the welding process is possible.

The transient behavior of node 102 is similar (Fig. 13) except that the decomposition product is martensite and it appears at a later time than the ferrite-bainite at node 98.

GENERAL COMMENTS

These authors submit that most of the elements of a relatively complete computer integrated weld microstructure system are in place and the essentials are contained in these two presentation (Parts A and B). Efficient solvers to decrease computing time and cost still merit additional study. In some cases the coupling is not as tight as it might be and further development in this area would be useful. A welding knowledge based system is under development to make this analysis capability accessible to designers of welds. There is also continuous improvement in post-processing graphics which is very important.

The next step in the metal physics of welding is to integrate microstructure dependent mechanical properties into the system. Eventually cracking (fracture), fatigue and creep mechanisms must be added to predict the behavior of welds in service.

CONCLUSIONS AND CONTRIBUTIONS

1. A finite element based system for computing transient microstructural changes during the welding process has been demonstrated.
2. The accuracy of the system was supported by comparing a computed and measured HAZ prior austenite grain sizes and microstructure fractions.
3. The concept and demonstration of microstructural contours to represent transient microstructure fields has been presented.

4. The capability of the system for tracking microstructural changes as a function of time and position was demonstrated.

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ABSTRACT

Controlling the Heat-Affected Zone Microstructure of Steel Welds

M.J.Bibby¹, J.A.Goldak¹ and J. Bowker²

It is well known that 80% of all steel tonnage is welded and that 80% of all failures in steel structures initiate at weld sites. Moreover, almost all weld site failures originate in the heat-affected zone (HAZ). Failure in the HAZ is not difficult to imagine when it is realized that brittle microstructures (martensite, bainite) form as a result of the thermal cycle; residual stresses often as high or higher than the yield level form as a result of thermal shrinkage; and hydrogen is pumped into the region from the heat source--almost ideal conditions for failure initiation.

It is the contention of these authors that the response of a steel to the welding process should be a major consideration in the development of new chemistries and thermomechanical processing procedures. Software designed at Carleton for this purpose will be described in this presentation. In particular a system for predicting HAZ microstructure based primarily on fundamental reaction rate principles is to be discussed. This approach will be compared with less comprehensive methods available for this purpose and with measured experimental results. Progress in this program will be discussed in terms of software as a tool for controlling microstructure in research and practice.

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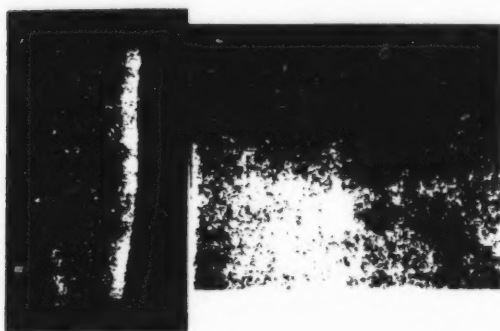
Bibby, M.J., Goldak J.A., and Bowker, J., "Controlling the Heat-Affected Zone Microstructure of Steel Welds", Seminar On Microstructural Engineering of Steel, IMRI, Boucherville, P.Q., September 1/88

THE ADDITION OF MICROSTRUCTURAL CALCULATIONS TO COMPUTATIONAL WELD MECHANICS

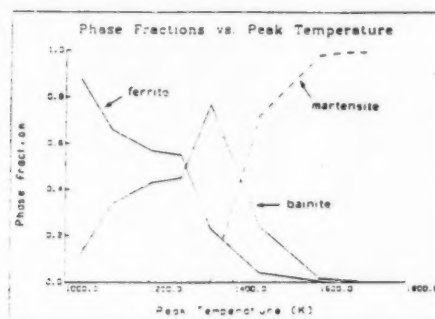
M.J. Bibby¹, C. Henwood¹, J. Goldak¹ and D. Watt²

It is now possible to compute the microstructural distribution in the heat-affected zone (HAZ) of a weld given the input welding parameters (current, voltage, welding speed), the joint and workpiece geometry, the chemistry of the base material, the initial conditions (preheat temperature and initial microstructure), and the boundary conditions (convective-radiative heat transfer coefficients). The computed residual microstructure distribution for a small bead-on-plate weld (heat input - 0.2 KJ/mm; plate thickness - 2.7 mm; plate chemistry C - 0.12, Mn - 0.91, Si - 0.16, Nb - 0.021, N - 0.011, S - 0.005, Al - 0.04) is shown in Figure 1 to demonstrate the capability of the system. In addition to this it is now possible to track the microstructure around the thermal cycle for any position in the neighbourhood of the weld.

The austenite decomposition kinetics algorithm used to do these computations is presented. Coupling this algorithm to either conventional "Rosenthal" or FEM heat transfer computations is described. Computed microstructural distributions are compared with experimental results as a means of evaluating the validity of the system.



A



B

Figure 1 (A) A deep penetration weld and a shallow weld shown to identify the heat-affected zone (HAZ); (B) the microstructure distribution across a small weld (welding conditions in text).

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A COMPUTER SYSTEM FOR PREDICTING THE RESPONSE OF STEEL CHEMISTRY TO THE WELDING PROCESS

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March 1, 1988

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Abstract

It has been said that over 80% of all steel tonnage is welded and that over 80% of all failures initiate at weld sites. In view of this it is not difficult to appreciate that "weldability" should occupy an important place in deciding steel chemistry. While there is a wealth of weldability research available in the literature to guide steelmakers, it is generally not in a "user friendly" form. A small computer system (PC or hand held for portability to a job site) that incorporates some of the more important weldability developments of the past several years is put forward in this presentation. A "user friendly" philosophy is described so that the system can be used routinely with little previous computer experience.

Input to the system consists of base metal chemistry, welding parameters (voltage, current, welding speed, preheat temperature, hydrogen level), workpiece and joint geometry, yield strength, and restraint level. The output consists of maximum heat-affected zone (HAZ) hardness, HAZ microstructure fractions (martensite level is particularly important) and preheat levels to avoid HAZ cracking.

Computed (and measured) results will be presented to show how the system can be used by a steelmaker to anticipate welding problems caused by either chemistry changes or chemistry variability. In addition, it is suggested that this same software could be used by steel manufacturers for guiding fabricator welding procedures to meet customer specifications. For example, a maximum HAZ hardness of 280 VPN is often imposed in the petroleum industry where a weld is to be exposed to sour gas situations. The software described in this presentation can be used as a guide to the welding process and parameters, and base metal chemistry to meet this specification.

Bibby, M.J., Bowker, J., Goldak, J.A., and Jefferson, I., "A Computer System for Predicting the Response of a New Steel Chemistry to the Welding Process, Steel Processing -- Process Integration, World Materials Congress, Chicago, Illinois, September 22-26, 1988

Integrating Microstructural Calculations Into computational Weld Mechanics

C. Henwood*, M. Bibby*, J. Goldak*, and D. Watt**

The principal objective of computational weld mechanics is to predict the mechanical behavior of a defect free weld on the one hand and the threshold appearance of crack defects on the other from the welding parameters including joint geometry, and base and filler metal composition. Once considered only a goal, such models are becoming operational. Obviously microstructural change driven by the weld thermal cycle must play a key role in these models.

Perhaps the most significant contribution in this area in recent years is the model suggested by Ion, Easterling and Ashby (1). While this work is an important development in the modelling of welding processes, it is based on "comparative kinetic principles" and as such experimental data are needed for a given joint composition before weld microstructures can be predicted for any alternative welding procedure. In addition, the model predicts only final (residual) microstructures while the full transient history is needed to model important cracking mechanisms.

Models are presented that support the computation of the microstructure field as a function of time and position from the thermal properties of the materials, joint shape, and boundary condition (welding parameters and environmental conditions). The transient temperature field is computed by finite element analysis (FEA) or by conventional means (Rosenthal model (2)). Materials principles are coupled to the transient field to track microstructural changes. Equilibrium is assumed on heating until grain growth in the austenite becomes significant. A modified version of the Ion, Easterling, Ashby kinetics is used to compute carbide/nitride dissolution (microalloy steels) and subsequent austenite grain growth. Avrami type ordinary differential equations (Kirkaldy, Venugopalan (3), Watt (4)) are integrated along a cooling curve (position dependent) to compute the formation of ferrite, bainite, pearlite and martensite.

Computed values of heat-affected zone (HAZ) grain size and microstructural phases present are compared with measured values for a low carbon microalloy steel. It is shown that the computed and measured results are in excellent agreement in spite of uncertainties in the measurements and in some of the data used for the computations. It is argued that such agreement is not fortuitous but expected because of the nature of the changes. In fact, evidence is provided to justify considerable faith in the computational system.

While the methodology and software has only been applied to short time high temperature weld thermal cycles, it can be applied to other thermo- or thermo-mechanical processes such as casting, or forging without much difficulty. Such a discussion is included in the presentation.

Henwood, C., Bibby, M.J., Goldak, J.A., and Watt, D., "Integrating Microstructural Calculations into Computational Weld Mechanics", 37th Canadian Metal Physics Conference, RMC (Kingston), June 3-5, 1987